



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

PDB ID : 1SMY
Title : Structural basis for transcription regulation by alarmone ppGpp
Authors : Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassylyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-03-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

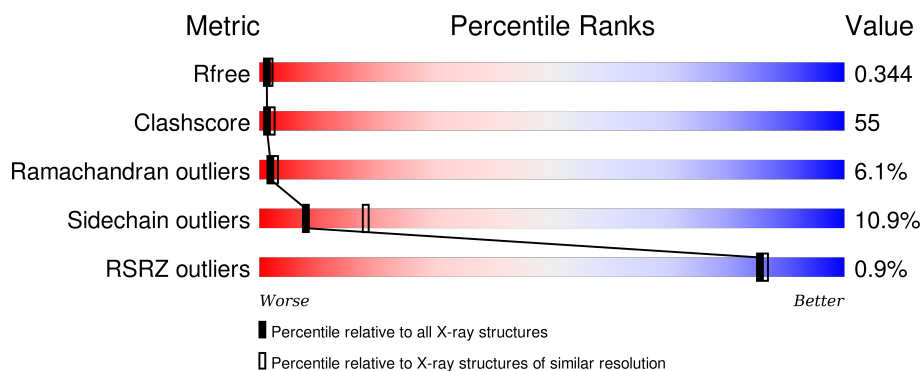
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div></div> <div> <div>21%</div> <div>44%</div> <div>8%</div> <div>27%</div> </div> </div>
1	B	315	<div> <div></div> <div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div> </div>
1	K	315	<div> <div></div> <div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div> </div>
1	L	315	<div> <div></div> <div> <div>23%</div> <div>46%</div> <div>.</div> <div>27%</div> </div> </div>
2	C	1119	<div> <div></div> <div> <div>28%</div> <div>59%</div> <div>12%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	A	9209	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 63021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA POLYMERASE OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called principal sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			
5	P	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			

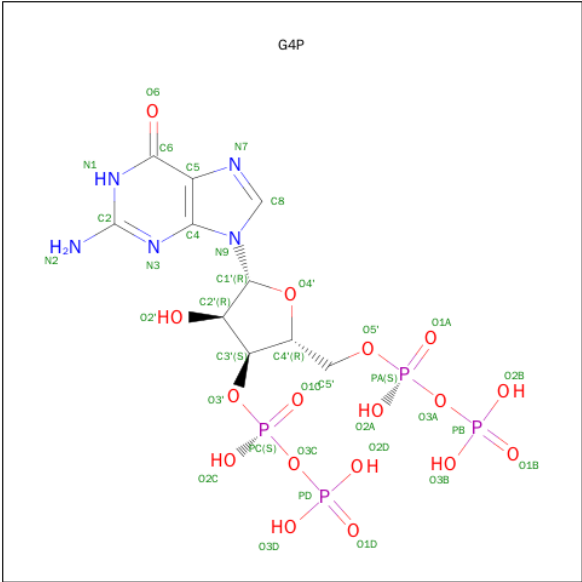
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	150	Total	Mg	0	0
			150	150		
6	E	17	Total	Mg	0	0
			17	17		
6	B	22	Total	Mg	0	0
			22	22		
6	C	92	Total	Mg	0	0
			92	92		
6	A	29	Total	Mg	0	0
			29	29		
6	N	2	Total	Mg	0	0
			2	2		
6	F	49	Total	Mg	0	0
			49	49		
6	M	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	N	2	Total	Zn	0	0
			2	2		

- Molecule 8 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	N	2	Total	C	N	O	P	0	0
			72	20	10	34	8		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	296	Total	O	0	0
			296	296		
9	B	307	Total	O	0	0
			307	307		
9	C	1308	Total	O	0	0
			1308	1308		
9	D	1745	Total	O	0	0
			1745	1745		
9	E	160	Total	O	0	0
			160	160		
9	F	619	Total	O	0	0
			619	619		
9	K	316	Total	O	0	0
			316	316		
9	L	341	Total	O	0	0
			341	341		
9	M	1401	Total	O	0	0
			1401	1401		
9	N	1794	Total	O	0	0
			1794	1794		
9	O	203	Total	O	0	0
			203	203		

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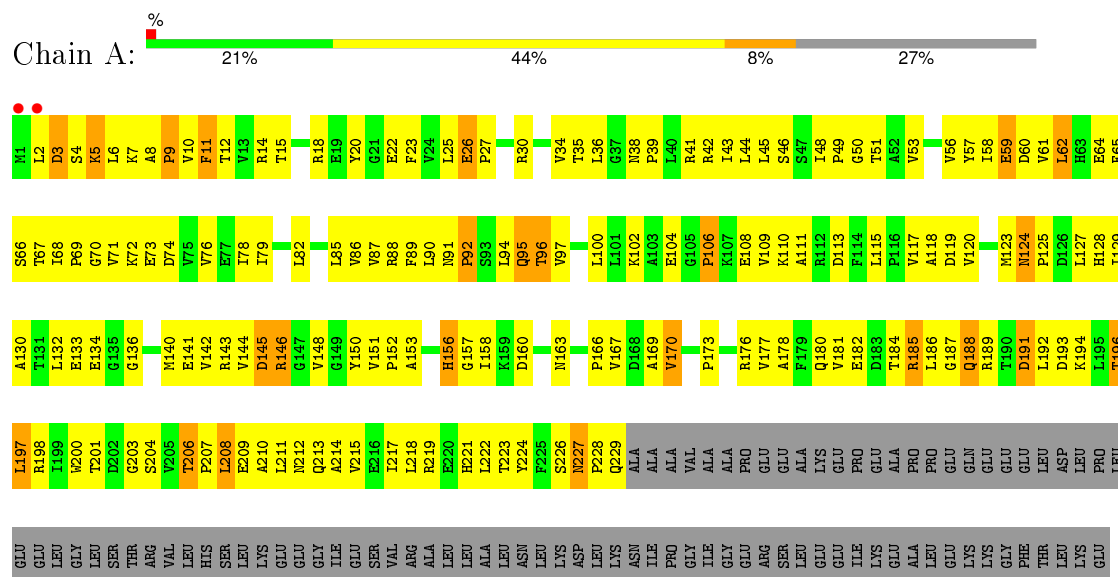
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	541	Total	O	0	0
			541	541		

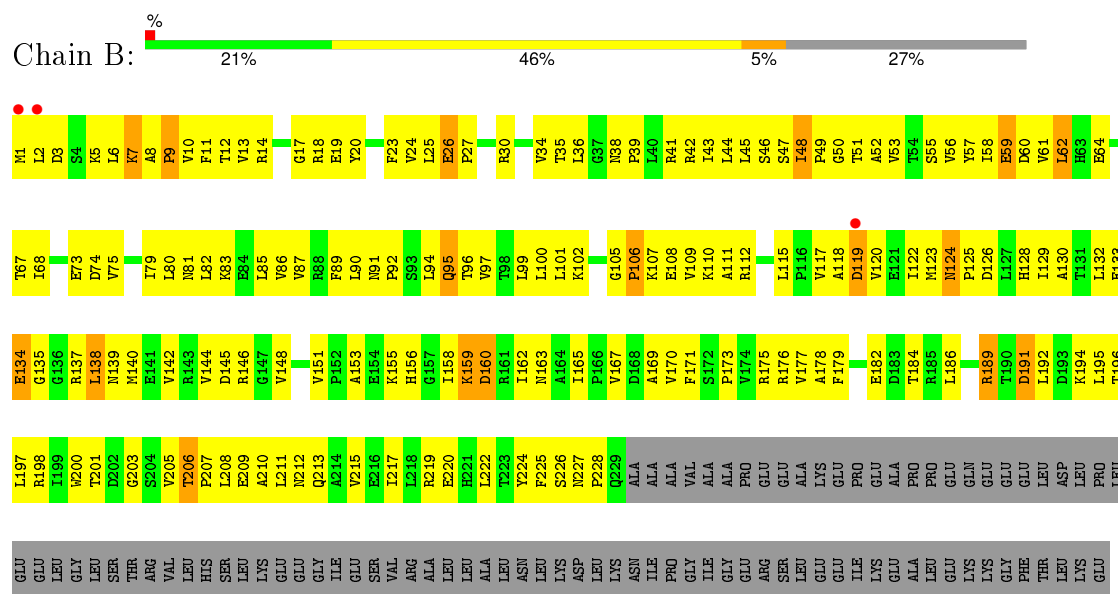
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

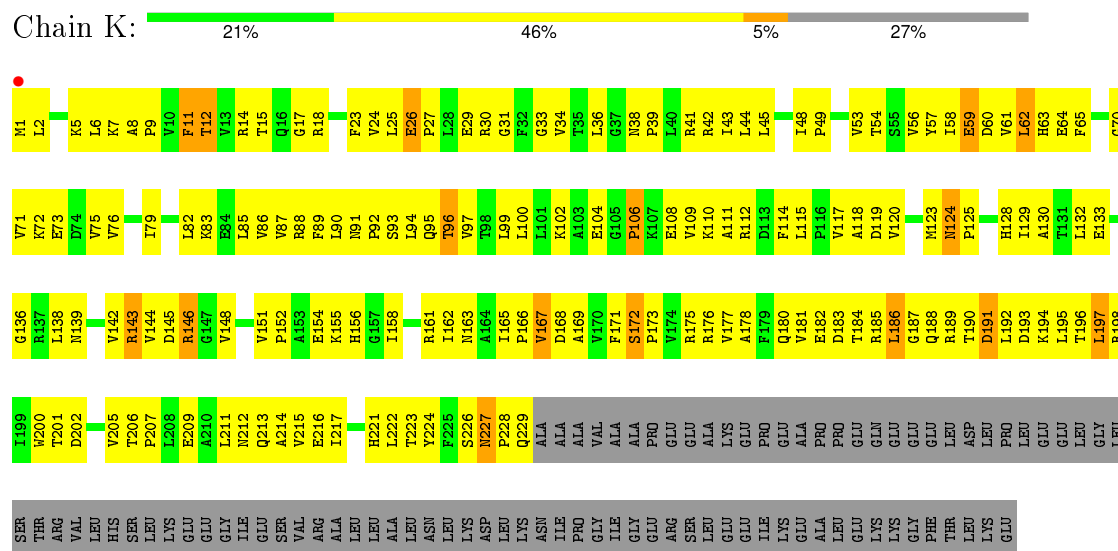
• Molecule 1: DNA-directed RNA polymerase alpha chain



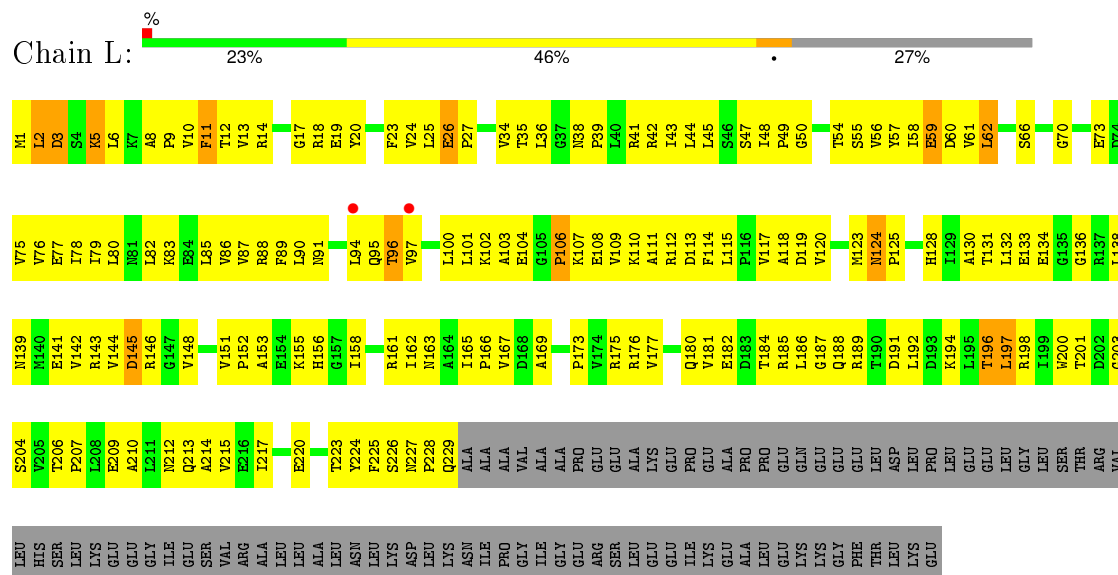
• Molecule 1: DNA-directed RNA polymerase alpha chain



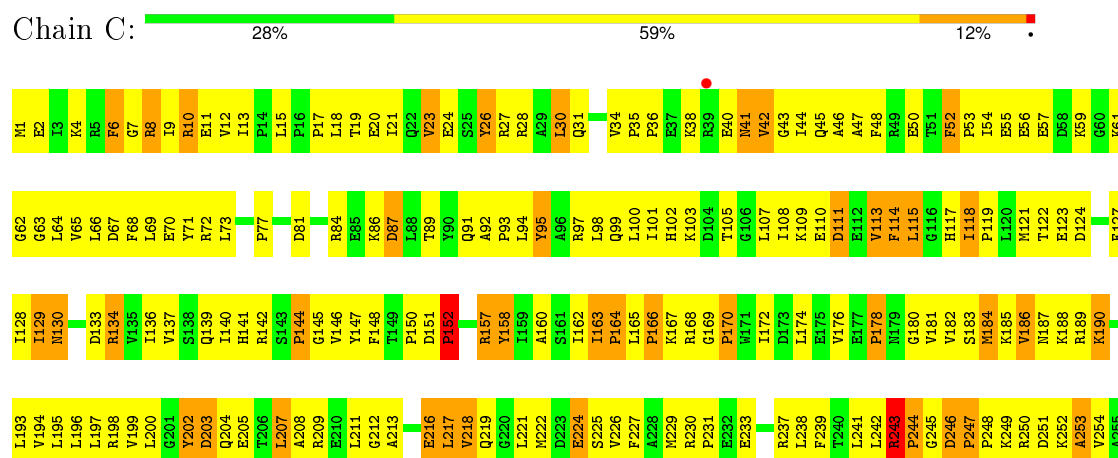
• Molecule 1: DNA-directed RNA polymerase alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain



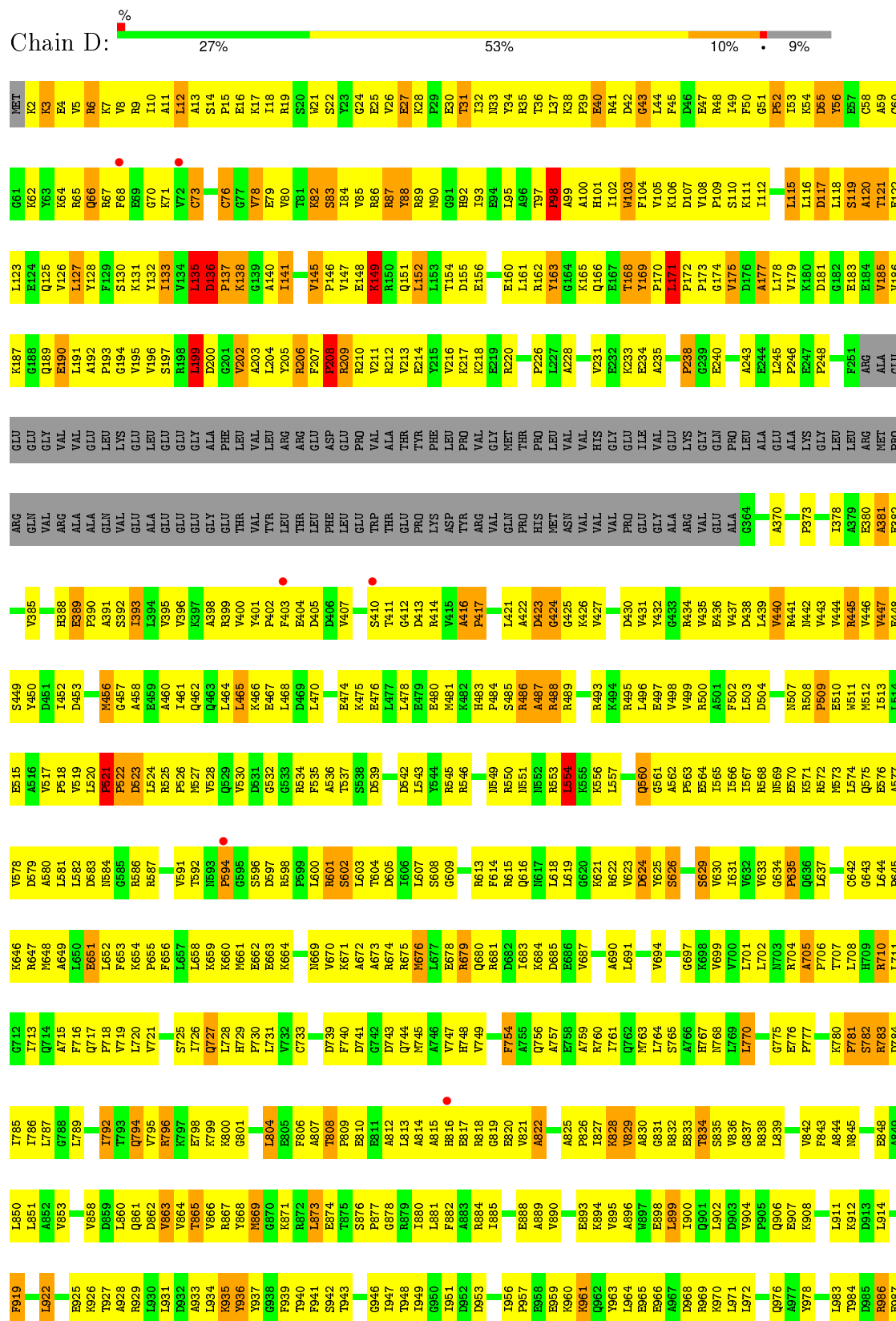
• Molecule 2: DNA-directed RNA polymerase beta chain





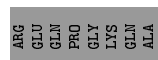
F1112	H1047	P982	I910	K846	L773	Y708	P641	P577	A515	I452	F385	H320	G259	L196	D133	G62
L1115	T1048	R983	E911	G847	L774	E709	R642	V578	R516	T463	F386	E321	L260	L197	R134	G63
R1119	L1049	E984	P912	V849	R775	E710	V643	M580	R518	S454		V322	L261	R198	V195	L64
	Q1050	G985	E913	V848	R776	E711	V644	M581	R519	S455	S389	D323	A262	R199	V136	G65
	E1051	P986	I914	A850	F777	E712	V645	T581	G519	A456	Q390	D324	D263	L201	V137	L66
	M1052	P987	K915	K851	F778	R713	G646	G582	E520	A457		I325	P264	G201	S138	D67
	L1053	V988	K916	L852	G779	K716	Q647	L583	P621	Y458	Q393	D826	R265	Y202	Q139	F68
	L1054	V989	L917	L853	E780		R648	E584	V522	A459	F394	H327	R266	D203	I140	L69
	T1055	G990	L918	P854	K781		V649	E585	I523	R460	K395	L328	Y267	Q204	H141	E70
	L1056	Q991	A919	V855	R782		R650	R586	S524	V461	D397		D268	E205	R142	Y71
	S1057	Q992	Q920	E856	A783		G651	V587	S525	D462	E397		L269	T206	S143	R72
	D1058	F993	Y925	M857	V784		G652	V588	P526	E463	T398	R332	G270	L207	P144	L73
	L1059		P926	M858	V785		G653	R589	E527	L464	I399	R333	G271	A208	G145	
	I1060	V996	G927	P859	K786		L654	D590	E528	G465		R334	A272	R209	V146	P76
	R1063	V997	G927	B860			L655				S402	T335	A273	E210	F147	
	H1064	V998	K928		S789		L656	A594	F531	R468	S403	T336	G274	E211	F148	E82
	A1065	H999	R929	G864	L790		D657	L595	M532	T469	L404	G337	Y275	G212	T149	R84
	A1066	M1000	K930	T865	R791		G658	Y596	D533	P470	R405	E338	K276	A213	P150	
	Y1067	V1001	G931	P866	V792		P659	A597	V534	Y471	H406	L339	A277		D151	
	L1068	E1002	E932	P867			A660	E598	S535	R472	R407	M340	E278	E216	P152	D87
	D1069	D1003		D868	G798		S730	E599	P536	R473	R408	T341	E279	L217		L88
	I1071	K1004	K937	V869	V799		L734	D600	K537	G476	R409	Q343	L281	Q219	R157	Y158
	D1074	M1005	K938	I870	V800		R802	G601	Q538			F344	G282	G220	T89	Y90
	Y1075	H1006	R939	M872	V801		R803	E602	V539	G477	S411	R345	G283	L221	I159	A92
	V1076	D1076	Y943	P873	T603			A604	S541	V478	A412	V346	L284	V222	A160	
	E1077	S1009	I944	L874			L668	R605	V542	V479	L413	G347	L285	D223	S161	P93
	E1078		R945	G875	D810		G669	V606	J543	T480	G414	E347	L286	E224	I162	L94
	P1079	P1012	R946	P876	G812		Q670	D607	T544	D481	P415	A349	S286	G232	I163	Y95
	S1080	G1013	A947	R771	G811		N671	G608	N545	E482	G416	R350	G287	S225	P164	A96
	L1081	S1014	E948	S878	V613		V672	N609	L546	V483	G417	V226	K288	V226	P165	R97
	P1082	L1015	I949	R879	G613		L673	R610	T547	V484	L418	F227	T289	P227	P166	L98
	E1083	L1016	R950	R880	K616		L674	R611	P548	Y485	R420	A352	L290	A228	K167	Q99
	S1084	T1017	G951	N881	P817		A675	V612	F549			R353	A291	R230	R168	L100
	Q1085	Q1018	L952	L882	G818		L676	V613	L550	A488	G424	V355	R292	E231	G169	I101
	R1086	G1019	V953	G883	V819		A747	R614	E551	T489	F425	M359		E232	W171	K103
	P1087	Q1020	T954	Q894	R820		P678	V615	H552	E491	D426	L360		E233	I172	
	L1088	L1021	P955	L885	E821		F679	E616	D553	D492	V427			A234	D173	
	V1089		G956	L886	V822		D680	D617	D544	R493	R428				L174	
	E1090	Q1026	K957	E887	V823			L620	A555	Y494		S363		R237	E175	K108
	L1092	G1028	T958	R889	V825			V621	N556	T495	H431			L238	V176	E110
	Q1093	G1029	E961	L892	Y826			E622	R557	A497	T433				E177	D111
	L1095	Q1030	Q962	A893	V827		A628	L625	N560	Q498	H434			L241	P178	E412
	A1096	F1032	K964		Q829			R626	G561	A499	T435			L242	R179	V113
	L1097	G1033	E965	F896	K830		L690	R627	S562	N500	G436			R243	V181	F114
	D1098	E1034	L966	L897	R831		S691	F628	N564	P501	R437			G245	G180	F115
	V1099	M1035	P967	G898	K832		E692	G634	O565	P502	L438			P246	V182	G116
	Q1100	E1036	L968	Q899	L833		E693	R629	T566	L503	Q439			D247	S183	H117
	T1101	V1037	Q969	R900			E694	R630	T566	E504				P248	M184	I118
	E1104	A1039	G970	Y901	D837		L695	N632	Q567	G505	B442			R249	K185	P119
	K1105	L1040	K971	S765	K838		L696	Q633	A568	N506	T443			R250	V186	L120
	D1106	E1041	D976	E766	L839		R697	R634	R507	R507	P444			D251	K188	
	N1107	P1042	G977	P767	G634		R698	T635	P570	L508	E445			K252	R189	D124
	P1108	Y1043	R978	T768	G699		F699	R636	L571	A510	Q446			A253	K190	F127
	L1109	G1044	T979	P769	Y700		T701	L637	L572	E511	M448			A254	F191	
	D1110		G980	E771				D638	A574	R512	L449			A255	P192	L128
	I1111	A1046		R772			R707	R640	A576	V514	L451			Y256	L193	I129
														Y258	P194	N130
															L195	

- Molecule 3: DNA-directed RNA polymerase beta' chain

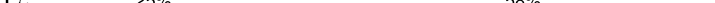


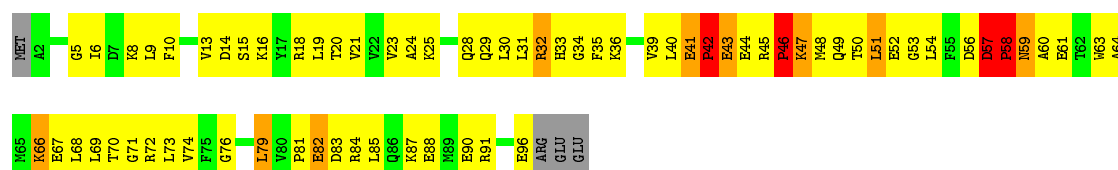


R1388	G1322	T1253	P1191	T1052	1992	A918	L850	Q788	V719	L652	G585	A516	D453	I393
L1389	Q1323	L1253	L1192	F1053	L993	F919	L851	L789	L720	F653	R586	V617	A454	L394
E1391	P1324	P1257	T1193	E1054	Q994	L920	A952	L792	W721	K654	R587	P518	R455	V395
G1392	L1325	R1258	C1194	V1055	L995	R921	V853	I792	E722	P655	G588	V519	R456	K397
G1393	T1326	L1262	Q1195	P1056	W996	L922	A854	Q794	G723	F656	P590	P521	A458	A398
V1394	R1327	L1262	P1120	V1057	W997	L922	A854	Q794	G723	F656	P590	P521	A458	A398
L1395	L1327	L1262	L1122	R1058	E998	E925	V858	R795	L728	L658	P594	P522	E459	R399
L1396	L1328	L1262	P1123	S1059	T999	R926	D859	R796	L728	K660	P594	P522	A460	V400
L1397	L1329	L1262	P1124	S1060	T999	R927	L860	R797	H729	K661	P594	P522	A460	V400
L1398	L1330	L1262	P1125	F1061	E1001	R928	Q861	R798	H729	K661	P594	P522	A460	V400
L1399	L1331	L1262	P1126	R1062	E1002	R929	Q862	R799	H729	K661	P594	P522	A460	V400
L1400	L1332	L1262	P1127	E1063	V1003	R930	V863	R800	V732	E662	P597	P526	Q462	F402
E1401	L1333	L1262	P1128	L1064	V1004	R931	V864	R801	V733	E663	P598	P527	L464	E404
L1402	L1334	L1262	P1129	L1065	Q1005	R935	V865	R801	V734	E664	P599	P528	L465	D405
L1403	L1335	L1262	P1130	T1066	Q1006	R936	V866	R802	V735	E665	P600	P535	L466	D406
L1404	L1336	L1262	P1131	L1067	V1007	R936	V867	R803	F736	M669	R601	P535	E467	V407
L1405	L1337	L1262	P1132	L1068	F1008	R937	V868	R804	F737	M670	R602	P536	L468	E408
L1406	L1338	L1262	P1133	L1069	F1009	R938	V869	R805	A738	M671	R603	P537	D469	V409
L1407	L1339	L1262	P1134	L1070	F1010	R939	V870	R806	D739	M672	R604	P538	L470	S410
L1408	L1340	L1262	P1135	L1071	F1011	R940	V871	R807	D740	M673	R605	P539	E471	T411
L1409	L1341	L1262	P1136	L1072	F1012	R941	V872	R808	D741	M674	R606	P540	L472	G412
L1410	L1342	L1262	P1137	L1073	F1013	R942	V873	R809	D742	M675	R607	P541	L473	G413
L1411	L1343	L1262	P1138	L1074	F1014	R943	V874	R810	D743	M676	R608	P542	L474	G414
L1412	L1344	L1262	P1139	L1075	F1015	R944	V875	R811	D744	M677	R609	P543	L475	R414
L1413	L1345	L1262	P1140	L1076	F1016	R945	V876	R812	D745	M678	R610	P544	L476	R415
L1414	L1346	L1262	P1141	L1077	F1017	R946	V877	R813	D746	M679	R611	P545	L477	A416
L1415	L1347	L1262	P1142	L1078	F1018	R947	V878	R814	D747	M680	R612	P546	L478	A417
L1416	L1348	L1262	P1143	L1079	F1019	R948	V879	R815	D748	M681	R613	P547	L479	A418
L1417	L1349	L1262	P1144	L1080	F1020	R949	V880	R816	D749	M682	R614	P548	L480	A419
L1418	L1350	L1262	P1145	L1081	F1021	R950	V881	R817	D750	M683	R615	P549	L481	A420
L1419	L1351	L1262	P1146	L1082	F1022	R951	V882	R818	D751	M684	R616	P550	L482	A421
L1420	L1352	L1262	P1147	L1083	F1023	R952	V883	R819	D752	M685	R617	P551	L483	A422
L1421	L1353	L1262	P1148	L1084	F1024	R953	V884	R820	D753	M686	R618	P552	L484	A423
L1422	L1354	L1262	P1149	L1085	F1025	R954	V885	R821	D754	M687	R619	P553	L485	A424
L1423	L1355	L1262	P1150	L1086	F1026	R955	V886	R822	D755	M688	R620	P554	L486	G424
L1424	L1356	L1262	P1151	L1087	F1027	R956	V887	R823	D756	M689	R621	P555	L487	G425
L1425	L1357	L1262	P1152	L1088	F1028	R957	V888	R824	D757	M690	R622	P556	L488	K426
L1426	L1358	L1262	P1153	L1089	F1029	R958	V889	R825	D758	M691	R623	P557	L489	K427
L1427	L1359	L1262	P1154	L1090	F1030	R959	V890	R826	D759	M692	R624	P558	L490	K428
L1428	L1360	L1262	P1155	L1091	F1031	R960	V891	R827	D760	M693	R625	P559	L491	A429
L1429	L1361	L1262	P1156	L1092	F1032	R961	V892	R828	D761	M694	R626	P560	L492	D430
L1430	L1362	L1262	P1157	L1093	F1033	R962	V893	R829	D762	M695	R627	P561	L493	D431
L1431	L1363	L1262	P1158	L1094	F1034	R963	V894	R830	D763	M696	R628	P562	L494	Y432
L1432	L1364	L1262	P1159	L1095	F1035	R964	V895	R831	D764	M697	R629	P563	L495	G433
L1433	L1365	L1262	P1160	L1096	F1036	R965	V896	R832	D765	M698	R630	P564	L496	R434
L1434	L1366	L1262	P1161	L1097	F1037	R966	V897	R833	D766	M699	R631	P565	L497	V435
L1435	L1367	L1262	P1162	L1098	F1038	R967	V898	R834	D767	M700	R632	P566	L498	V436
L1436	L1368	L1262	P1163	L1099	F1039	R968	V899	R835	D768	M701	R633	P567	L499	V437
L1437	L1369	L1262	P1164	L1100	F1040	R969	V900	R836	D769	M702	R634	P568	L500	D438
L1438	L1370	L1262	P1165	L1101	F1041	R970	V901	R837	D770	M703	R635	P569	L501	L439
L1439	L1371	L1262	P1166	L1102	F1042	R971	V902	R838	D771	M704	R636	P570	L502	V440
L1440	L1372	L1262	P1167	L1103	F1043	R972	V903	R839	D772	M705	R637	P571	L503	R441
L1441	L1373	L1262	P1168	L1104	F1044	R973	V904	R840	D773	M706	R638	P572	L504	R442
L1442	L1374	L1262	P1169	L1105	F1045	R974	V905	R841	D774	M707	R639	P573	L505	R443
L1443	L1375	L1262	P1170	L1106	F1046	R975	V906	R842	D775	M708	R640	P574	L506	V444
L1444	L1376	L1262	P1171	L1107	F1047	R976	V907	R843	D776	M709	R641	P575	L507	V445
L1445	L1377	L1262	P1172	L1108	F1048	R977	V908	R844	D777	M710	R642	P576	L508	R446
L1446	L1378	L1262	P1173	L1109	F1049	R978	V909	R845	D778	M711	R643	P577	L509	V447
L1447	L1379	L1262	P1174	L1110	F1050	R979	V910	R846	D779	M712	R644	P578	L510	V448
L1448	L1380	L1262	P1175	L1111	F1051	R980	V911	R847	D780	M713	R645	P579	L511	E448
L1449	L1381	L1262	P1176	L1112	F1052	R981	V912	R848	D781	M714	R646	P580	L512	S449
L1450	L1382	L1262	P1177	L1113	F1053	R982	V913	R849	D782	M715	R647	P581	L513	E450
L1451	L1383	L1262	P1178	L1114	F1054	R983	V914	R850	D783	M716	R648	P582	L514	D451
L1452	L1384	L1262	P1179	L1115	F1055	R984	V915	R851	D784	M717	R649	P583	L515	E452
L1453	L1385	L1262	P1180	L1116	F1056	R985	V916	R852	D785	M718	R650	P584	L516	E453
L1454	L1386	L1262	P1181	L1117	F1057	R986	V917	R853	D786	M719	R651	P585	L517	E454
L1455	L1387	L1262	P1182	L1118	F1058	R987	V918	R854	D787	M720	R652	P586	L518	E455
L1456	L1388	L1262	P1183	L1119	F1059	R988	V919	R855	D788	M721	R653	P587	L519	E456
L1457	L1389	L1262	P1184	L1120	F1060	R989	V920	R856	D789	M722	R654	P588	L520	E457
L1458	L1390	L1262	P1185	L1121	F1061	R990	V921	R857	D790	M723	R655	P589	L521	E458
L1459	L1391	L1262	P1186	L1122	F1062	R991	V922	R858	D791	M724	R656	P590	L522	E459
L1460	L1392	L1262	P1187	L1123	F1063	R992	V923	R859	D792	M725	R657	P591	L523	E460
L1461	L1393	L1262	P1188	L1124	F1064	R993	V924	R860	D793	M726	R658	P592	L524	E461
L1462	L1394	L1262	P1189	L1125	F1065	R994	V925	R861	D794	M727	R659	P593	L525	E462
L1463	L1395	L1262	P1190	L1126	F1066	R995	V926	R862	D795	M728	R660	P594	L526	E463
L1464	L1396	L1262	P1191	L1127	F1067	R996	V927	R863	D796	M729	R661	P595	L527	E464
L1465	L1397	L1262	P1192	L1128	F1068	R997	V928	R864	D797	M730	R662	P596	L528	E465
L1466	L1398	L1262	P1193	L1129	F1069	R998	V929	R865	D798	M731	R663	P597	L529	E466
L1467	L1399	L1262	P1194	L1130	F1070	R999	V930	R866	D799	M732	R664	P598	L530	E467
L1468	L1400	L1262	P1195	L1131	F1071	R1000	V931	R867	D800	M733	R665	P599	L531	E468
L1469	L1401	L1262	P1196	L1132	F1072	R1001	V932	R868	D801	M734	R666	P600	L532	E469
L1470	L1402	L1262	P1197	L1133	F1073	R1002	V933	R869	D802	M735	R667	P601	L533	E470
L1471	L1403	L1262	P1198	L1134	F1074	R1003	V934	R870	D803	M736	R668	P602	L534	E471
L1472	L1404	L1262	P1199	L1135	F1075	R1004	V935	R871	D804	M737	R669	P603	L535	E472
L1473	L1405	L1262	P1200	L1136	F1076	R1005	V936	R872	D805	M738	R670	P604	L536	E473
L1474	L1406	L1262	P1201	L1137	F1077	R1006	V937	R873	D806	M739	R671	P605	L537	E474
L1475	L1407	L1262	P1202	L1138	F1078	R1007	V938	R874	D807	M740	R672	P606	L538	E475
L1476	L1408	L1262	P1203	L1139	F1079	R1008	V939	R875	D808	M741	R673	P607	L539	E476
L1477	L1409	L1262	P1204	L1140	F1080	R1009	V940	R876	D809	M742	R674	P608	L540	E477
L1478	L1410	L1262	P1205	L1141	F1081	R1010	V941	R877	D810	M743	R675	P609	L541	E478
L1479	L1411	L1262	P1206	L1142	F1082	R1011	V942	R878	D811	M744	R676	P610	L542	E479
L1480	L1412	L1262	P1207	L1143	F1083	R1012	V943	R879	D812	M745	R677	P611	L543	E480
L1481	L1413	L1262	P1208	L1144	F1084	R1013	V944	R880	D813					



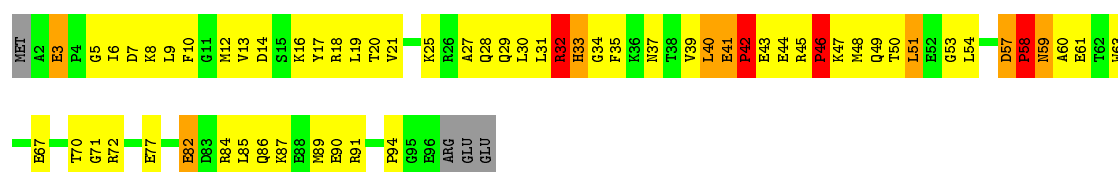
- Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

Chain E:  25% 58% 9% . .



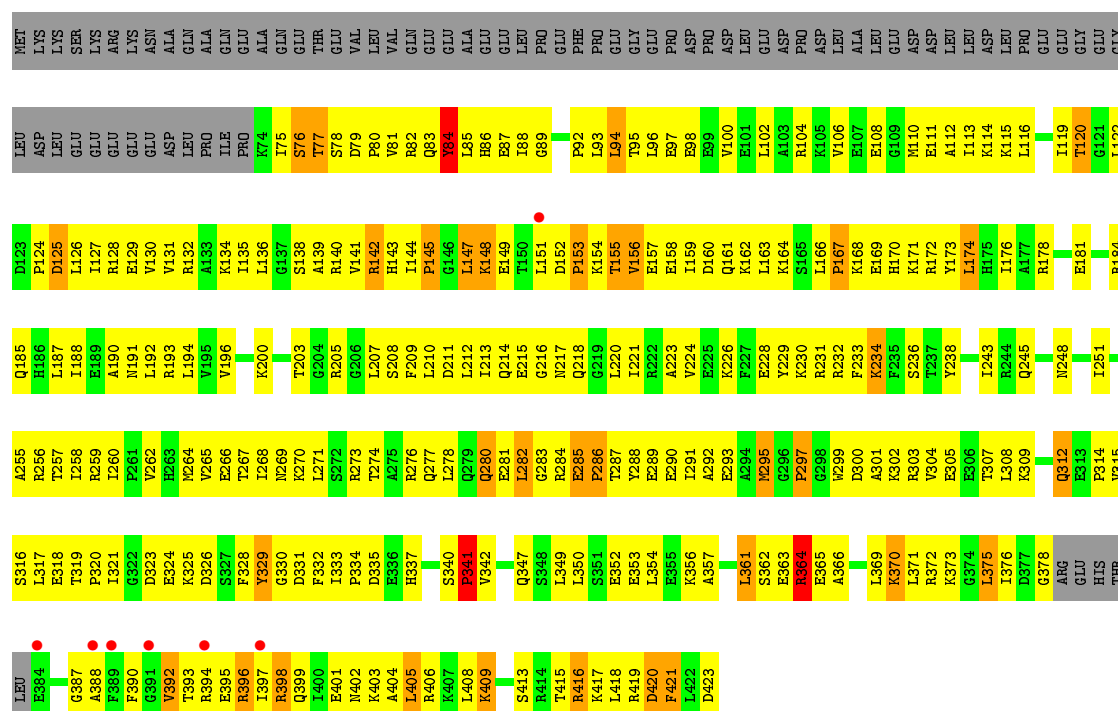
- Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

Chain O: 33% 51% 8% . .



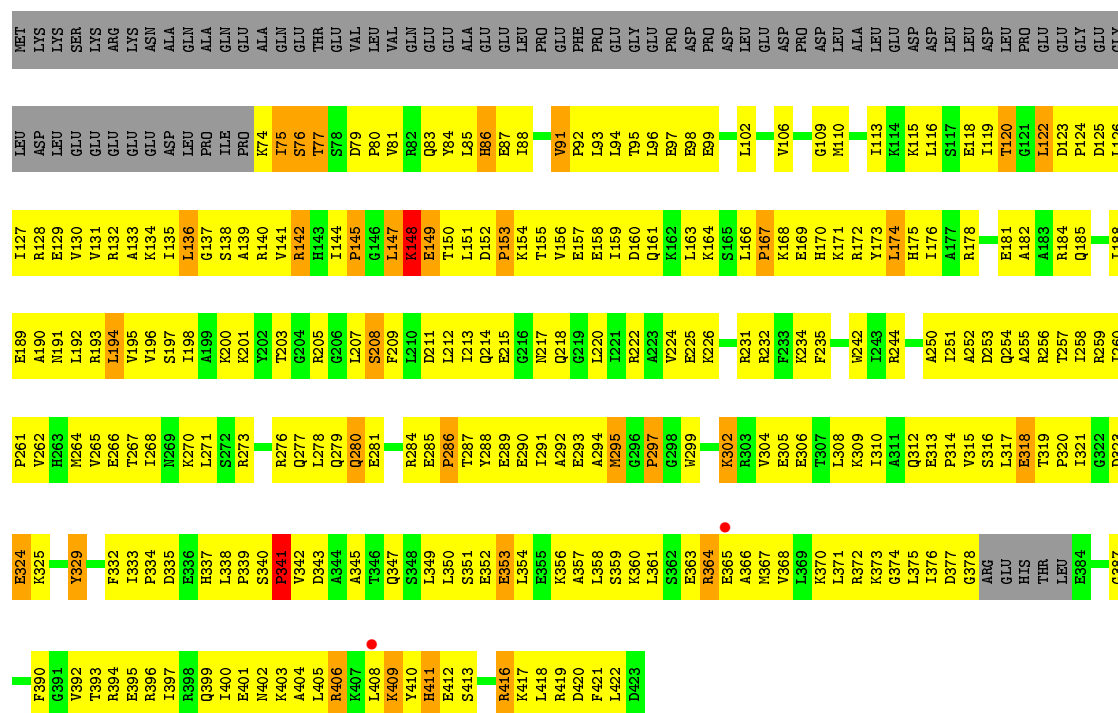
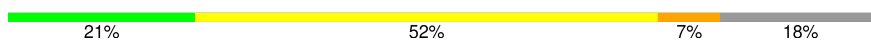
- Molecule 5: principal sigma factor

Chain F: 



- Molecule 5: principal sigma factor

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 50.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (50.12-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.266 0.305 , 0.344	Depositor DCC
R_{free} test set	14873 reflections (3.77%)	DCC
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.086 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 409145 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63021	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/1838	0.70	0/2498
1	B	0.68	0/1838	0.68	0/2498
1	K	0.68	0/1838	0.72	1/2498 (0.0%)
1	L	0.68	0/1838	0.67	1/2498 (0.0%)
2	C	0.75	0/8996	0.79	4/12164 (0.0%)
2	M	0.74	0/8996	0.78	4/12164 (0.0%)
3	D	0.74	0/10975	0.81	10/14836 (0.1%)
3	N	0.73	0/10975	0.81	14/14836 (0.1%)
4	E	0.74	0/783	0.81	0/1054
4	O	0.75	0/783	0.81	0/1054
5	F	0.65	0/2811	0.75	1/3781 (0.0%)
5	P	0.64	0/2811	0.74	1/3781 (0.0%)
All	All	0.72	0/54482	0.78	36/73662 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	243	ARG	C-N-CD	-9.21	100.34	120.60
3	D	199	LEU	CA-CB-CG	-8.95	94.72	115.30
3	N	199	LEU	CA-CB-CG	-8.85	94.94	115.30
1	K	197	LEU	CA-CB-CG	8.22	134.21	115.30
2	C	243	ARG	C-N-CD	-7.23	104.69	120.60
3	D	804	LEU	CA-CB-CG	6.65	130.59	115.30
5	P	136	LEU	CA-CB-CG	6.29	129.78	115.30
2	M	950	LEU	CA-CB-CG	6.07	129.27	115.30
5	F	84	TYR	CA-CB-CG	6.06	124.92	113.40
3	N	783	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	D	783	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	N	813	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	197	LEU	CA-CB-CG	5.56	128.10	115.30
2	M	193	LEU	CA-CB-CG	5.53	128.02	115.30
3	N	1290	LEU	CA-CB-CG	5.53	128.01	115.30
3	D	238	PRO	N-CA-CB	5.48	109.88	103.30
3	D	554	LEU	CA-CB-CG	5.44	127.81	115.30
2	M	244	PRO	CA-N-CD	-5.42	103.91	111.50
3	N	1201	CYS	CA-CB-SG	-5.36	104.34	114.00
2	C	853	LEU	CA-CB-CG	5.34	127.58	115.30
3	D	73	CYS	CA-CB-SG	5.32	123.58	114.00
3	N	1068	LEU	CA-CB-CG	-5.29	103.12	115.30
2	C	269	LEU	CA-CB-CG	5.27	127.42	115.30
3	N	171	LEU	CA-CB-CG	5.26	127.40	115.30
3	N	238	PRO	N-CA-CB	5.22	109.57	103.30
3	N	1209	LEU	N-CA-C	-5.18	97.02	111.00
3	N	705	ALA	C-N-CD	5.17	139.25	128.40
3	D	226	PRO	N-CA-CB	5.16	109.49	103.30
3	D	248	PRO	N-CA-CB	5.14	109.47	103.30
3	D	1209	LEU	N-CA-C	-5.11	97.21	111.00
3	N	710	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	N	373	PRO	N-CA-CB	5.09	109.41	103.30
2	C	559	LEU	CA-CB-CG	5.09	127.00	115.30
3	D	171	LEU	CA-CB-CG	5.08	126.99	115.30
3	N	136	ASP	C-N-CD	5.08	139.07	128.40
3	N	226	PRO	N-CA-CB	5.07	109.38	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	211	0
1	B	1806	0	1861	191	0
1	K	1806	0	1861	196	0
1	L	1806	0	1861	183	0
2	C	8828	0	8933	1013	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	8828	0	8933	1065	0
3	D	10797	0	10873	1260	0
3	N	10797	0	10873	1227	0
4	E	769	0	775	104	0
4	O	769	0	775	96	0
5	F	2770	0	2844	327	0
5	P	2770	0	2844	363	0
6	A	29	0	0	0	0
6	B	22	0	0	0	0
6	C	92	0	0	0	0
6	D	150	0	0	0	0
6	E	17	0	0	0	0
6	F	49	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	N	72	0	22	9	0
9	A	296	0	0	67	0
9	B	307	0	0	66	0
9	C	1308	0	0	281	0
9	D	1745	0	0	322	0
9	E	160	0	0	37	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	64	0
9	M	1401	0	0	325	0
9	N	1794	0	0	330	0
9	O	203	0	0	33	0
9	P	541	0	0	96	0
All	All	63021	0	54316	5952	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (5952) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.28	1.11
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.33	1.10
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:9100:G4P:H5"	8:N:9100:G4P:H8	1.14	1.09
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.35	1.08
2:C:328:LEU:HD13	2:C:433:THR:HB	1.37	1.07
3:D:95:LEU:HD11	3:D:517:VAL:HG23	1.34	1.05
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.40	1.04
5:P:278:LEU:HB3	5:P:286:PRO:HG2	1.38	1.03
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.39	1.01
3:N:908:LYS:HB2	3:N:1027:GLY:HA3	1.41	1.01
3:N:172:PRO:HB3	3:N:178:LEU:HB3	1.43	1.01
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.24	1.00
2:M:829:GLN:HE21	2:M:831:ARG:HD3	1.24	1.00
2:M:892:LEU:HD23	2:M:918:LEU:HD11	1.41	1.00
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.42	0.99
3:D:984:THR:HG22	3:D:987:GLU:HG3	1.44	0.99
2:M:546:LEU:HD12	2:M:565:GLN:HE22	1.26	0.99
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.42	0.98
3:D:1209:LEU:HD12	3:D:1210:SER:H	1.29	0.98
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.43	0.98
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.47	0.97
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.48	0.96
3:D:489:ARG:HG3	3:D:493:ARG:HH12	1.29	0.95
3:D:1432:LYS:HD2	3:D:1433:SER:H	1.28	0.95
4:O:40:LEU:HD21	4:O:67:GLU:HA	1.46	0.95
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.48	0.95
3:D:1389:LEU:HG	3:D:1390:LEU:HD23	1.48	0.94
2:C:627:ARG:H	2:C:627:ARG:HE	1.05	0.94
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.48	0.94
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.47	0.94
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.48	0.94
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.47	0.94
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.50	0.94
5:F:278:LEU:HB3	5:F:286:PRO:HG2	1.48	0.94
3:D:1388:ARG:H	3:D:1388:ARG:HD2	1.29	0.93
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.51	0.93
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.33	0.93
2:M:777:ILE:HG23	5:P:409:LYS:HB2	1.50	0.93
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.51	0.92
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.49	0.92
3:D:787:LEU:HD21	3:D:947:ILE:HD11	1.49	0.92
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.52	0.92
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.33	0.91
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.51	0.91
3:D:489:ARG:HE	3:D:493:ARG:HH22	1.18	0.91
2:M:95:TYR:HD2	2:M:114:PHE:HB3	1.37	0.91
3:N:32:ILE:HD12	3:N:527:MET:HG2	1.53	0.91
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.52	0.90
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.52	0.90
2:M:331:ARG:HH12	2:M:427:VAL:HG13	1.37	0.90
2:C:952:LEU:HD12	2:C:969:GLN:HE22	1.34	0.90
3:N:1137:ARG:H	3:N:1137:ARG:HD2	1.35	0.89
2:C:945:ARG:HB2	2:C:945:ARG:HH11	1.36	0.89
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.54	0.89
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.53	0.89
3:D:154:THR:HB	9:D:3232:HOH:O	1.72	0.89
3:D:87:ARG:HG3	3:D:88:TYR:H	1.38	0.89
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.38	0.89
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.34	0.89
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.55	0.89
2:C:405:ARG:HH12	2:C:409:ARG:HH21	1.21	0.88
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.56	0.88
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.52	0.88
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.56	0.88
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.53	0.88
2:C:207:LEU:HD22	2:C:221:LEU:HD21	1.56	0.88
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.39	0.88
2:C:938:LYS:HB3	2:C:939:ARG:HH21	1.39	0.88
9:K:4396:HOH:O	2:M:978:ARG:HA	1.74	0.87
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.55	0.87
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.55	0.87
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.56	0.87
3:N:65:ARG:HB2	5:P:375:LEU:HA	1.54	0.87
2:C:941:VAL:HA	2:C:944:LEU:HD12	1.54	0.87
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.56	0.86
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.56	0.86
2:M:148:PHE:HB3	2:M:313:LEU:HD22	1.57	0.86
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.55	0.86
5:P:252:ALA:HB1	5:P:265:VAL:HG21	1.58	0.86
3:N:646:LYS:HA	3:N:720:LEU:HD22	1.55	0.86
3:N:98:PRO:HG2	3:N:462:GLN:HE22	1.38	0.86
5:P:135:ILE:HD11	5:P:178:ARG:HD3	1.58	0.85
2:C:841:ASN:HD21	2:C:845:ASN:H	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.58	0.85
2:M:442:GLU:HG2	2:M:454:SER:HB2	1.58	0.85
3:D:119:SER:HB2	3:D:123:LEU:H	1.41	0.85
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.57	0.85
3:N:172:PRO:HG3	3:N:178:LEU:HD22	1.59	0.85
3:D:44:LEU:HB2	9:D:9962:HOH:O	1.77	0.85
3:N:1389:LEU:H	3:N:1389:LEU:HD23	1.40	0.85
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.57	0.85
3:N:1090:ASP:HB3	3:N:1093:TYR:HB2	1.57	0.85
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.58	0.85
8:N:9100:G4P:C8	8:N:9100:G4P:H5"	2.04	0.84
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.57	0.84
2:M:1097:LEU:HD22	2:M:1097:LEU:H	1.42	0.84
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.57	0.84
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.59	0.84
3:N:67:ARG:HD3	5:P:375:LEU:HD11	1.58	0.84
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.59	0.84
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.60	0.84
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.60	0.84
3:D:679:ARG:HH12	3:D:681:ARG:HD2	1.44	0.83
3:D:85:VAL:HB	3:D:89:ARG:HE	1.44	0.83
2:M:536:PRO:HB3	2:M:906:PHE:HD1	1.39	0.83
2:M:265:ARG:HA	9:M:9500:HOH:O	1.78	0.83
3:N:119:SER:H	3:N:123:LEU:HD22	1.43	0.83
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.61	0.83
1:L:206:THR:HG22	1:L:209:GLU:HB2	1.61	0.83
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	1.61	0.83
2:M:136:ILE:HA	9:M:9466:HOH:O	1.79	0.82
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.61	0.82
5:P:142:ARG:HB3	5:P:142:ARG:HH11	1.42	0.82
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.41	0.82
3:D:890:VAL:HG13	3:D:926:LYS:HD3	1.60	0.82
2:M:266:ARG:HD3	2:M:288:ARG:HH12	1.44	0.82
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.62	0.82
3:D:6:ARG:NH1	3:D:6:ARG:HB3	1.95	0.82
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.59	0.82
2:M:841:ASN:HD21	2:M:845:ASN:H	1.23	0.81
2:M:498:GLN:HG3	2:M:516:ARG:HH21	1.44	0.81
4:E:76:GLY:HA3	4:E:79:LEU:HD13	1.62	0.81
3:N:141:ILE:HD13	3:N:450:TYR:H	1.45	0.81
2:M:650:ARG:H	2:M:650:ARG:HE	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.61	0.81
3:D:212:ARG:HB2	3:D:445:ARG:HH22	1.45	0.81
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.62	0.81
1:A:180:GLN:HE22	2:C:934:PHE:HB2	1.44	0.81
2:M:89:THR:HG23	2:M:129:ILE:HA	1.62	0.81
2:C:238:LEU:HA	2:C:241:LEU:HD12	1.63	0.81
3:N:175:VAL:HG12	9:N:2205:HOH:O	1.80	0.81
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.61	0.81
3:N:422:ALA:HB1	5:P:178:ARG:NH1	1.96	0.81
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.60	0.81
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.62	0.81
2:C:89:THR:HG23	2:C:129:ILE:HA	1.59	0.81
2:C:244:PRO:HD2	2:C:245:GLY:H	1.42	0.81
2:C:139:GLN:HE22	2:C:415:PRO:HD2	1.45	0.81
1:K:112:ARG:HG2	9:K:1330:HOH:O	1.80	0.81
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.61	0.81
2:C:1054:THR:HA	9:C:9720:HOH:O	1.80	0.81
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.62	0.81
3:N:565:ILE:H	3:N:565:ILE:HD12	1.45	0.81
4:E:9:LEU:HB3	4:E:19:LEU:HD21	1.63	0.81
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.61	0.81
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.61	0.81
3:D:780:LYS:HD3	3:D:912:LYS:HD3	1.61	0.81
3:N:800:LYS:HG2	3:N:829:VAL:HG12	1.62	0.81
2:C:704:HIS:HB3	2:C:829:GLN:HE21	1.45	0.81
3:N:414:ARG:HD3	9:N:9486:HOH:O	1.81	0.80
3:N:116:LEU:HB3	3:N:118:LEU:HD13	1.63	0.80
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.61	0.80
3:D:704:ARG:HD2	3:D:705:ALA:H	1.47	0.80
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.64	0.80
2:C:971:LYS:HA	2:C:988:VAL:HA	1.62	0.80
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.61	0.80
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.64	0.80
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.61	0.80
2:M:238:LEU:HD23	2:M:241:LEU:HD12	1.64	0.80
3:N:899:LEU:HB2	3:N:917:GLN:HG2	1.61	0.80
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.61	0.80
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.64	0.80
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.63	0.80
2:M:192:PRO:HB2	2:M:195:LEU:HD13	1.63	0.80
3:D:210:ARG:HD2	3:D:398:ALA:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.46	0.80
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.64	0.80
2:M:340:MET:HA	9:M:2031:HOH:O	1.82	0.79
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.63	0.79
3:N:654:LYS:HD3	3:N:674:ARG:HH12	1.45	0.79
1:B:132:LEU:HD11	1:B:138:LEU:HD12	1.64	0.79
3:D:87:ARG:O	3:D:521:PRO:HB3	1.82	0.79
3:D:87:ARG:HG3	3:D:88:TYR:N	1.97	0.79
2:M:331:ARG:HB2	9:M:9297:HOH:O	1.81	0.79
1:L:58:ILE:HB	1:L:61:VAL:HB	1.63	0.79
2:M:650:ARG:HG2	2:M:653:ASP:HB2	1.65	0.79
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.63	0.79
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.62	0.79
3:N:87:ARG:O	3:N:521:PRO:HB3	1.83	0.79
3:D:427:VAL:HG23	9:D:2135:HOH:O	1.83	0.79
3:N:87:ARG:HA	9:N:9625:HOH:O	1.83	0.79
2:C:290:LEU:HD13	2:C:290:LEU:H	1.47	0.79
5:F:266:GLU:HA	5:F:269:ASN:HD22	1.47	0.79
8:N:9100:G4P:H8	8:N:9100:G4P:C5'	2.08	0.79
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.65	0.79
2:M:134:ARG:HA	9:M:9211:HOH:O	1.82	0.78
1:L:80:LEU:HD13	3:N:842:VAL:HG12	1.65	0.78
2:C:93:PRO:HA	9:C:9603:HOH:O	1.83	0.78
5:F:312:GLN:HB2	9:F:2094:HOH:O	1.84	0.78
2:C:755:LEU:HD12	2:C:825:VAL:HG11	1.64	0.78
3:N:135:LEU:HD11	3:N:452:ILE:HD11	1.64	0.78
2:C:325:ILE:HD12	2:C:325:ILE:H	1.47	0.78
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.65	0.78
2:C:24:GLU:HB3	2:C:28:ARG:HH12	1.48	0.78
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.65	0.78
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.65	0.78
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.66	0.78
2:C:333:ILE:HG22	2:C:465:GLY:HA2	1.65	0.78
2:M:650:ARG:H	2:M:650:ARG:NE	1.81	0.78
3:D:1328:GLY:HA3	9:D:2287:HOH:O	1.84	0.78
5:F:164:LYS:HA	5:F:171:LYS:NZ	1.98	0.78
3:D:759:ALA:HA	3:D:763:MET:HE2	1.66	0.78
2:C:42:VAL:HG12	2:C:43:GLY:H	1.48	0.78
3:D:775:GLY:HA3	3:D:1145:TYR:HE1	1.49	0.78
2:M:164:PRO:HA	2:M:266:ARG:HH22	1.47	0.78
2:C:66:LEU:HB2	9:C:2120:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:90:MET:HG2	3:D:521:PRO:HD3	1.65	0.78
2:M:314:THR:HG22	9:M:2325:HOH:O	1.84	0.78
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.66	0.78
3:D:978:TYR:HA	9:D:2242:HOH:O	1.83	0.77
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.64	0.77
1:K:34:VAL:HG21	9:M:9419:HOH:O	1.84	0.77
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.66	0.77
3:D:972:LEU:HG	3:D:976:GLN:HE22	1.47	0.77
1:B:58:ILE:HB	1:B:61:VAL:HB	1.66	0.77
5:F:214:GLN:HA	5:F:217:ASN:HD22	1.48	0.77
3:D:553:ARG:HH21	5:F:215:GLU:HG2	1.48	0.77
1:K:195:LEU:HG	9:K:1736:HOH:O	1.84	0.77
2:M:42:VAL:HG12	2:M:43:GLY:H	1.49	0.77
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.65	0.77
3:D:907:GLU:HA	9:D:9566:HOH:O	1.83	0.77
2:M:66:LEU:HD13	2:M:100:LEU:HB3	1.64	0.77
2:C:715:THR:HG22	2:C:717:LEU:H	1.47	0.77
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.67	0.77
3:D:1388:ARG:N	3:D:1388:ARG:HH11	1.83	0.77
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.67	0.77
4:O:48:MET:HB2	4:O:54:LEU:HB2	1.67	0.77
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.67	0.77
3:D:500:ARG:NH2	3:D:1388:ARG:HE	1.83	0.77
2:M:164:PRO:HA	2:M:266:ARG:HH12	1.49	0.77
2:M:971:LYS:HA	2:M:988:VAL:HA	1.65	0.77
3:N:119:SER:HB2	3:N:123:LEU:H	1.49	0.77
1:K:136:GLY:HA3	9:K:1268:HOH:O	1.85	0.77
1:K:53:VAL:HG12	1:K:167:VAL:HG21	1.67	0.77
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.67	0.77
3:N:783:ARG:NH1	3:N:1029:ARG:HG2	2.00	0.76
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.65	0.76
2:C:575:GLN:H	2:C:667:ALA:HB1	1.49	0.76
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.67	0.76
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.65	0.76
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.67	0.76
2:C:689:VAL:HG21	9:C:9624:HOH:O	1.86	0.76
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.66	0.76
3:D:777:PRO:HA	9:D:9581:HOH:O	1.85	0.76
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.50	0.76
3:D:583:ASP:OD1	3:D:604:THR:HB	1.84	0.76
5:F:287:THR:HG23	5:F:289:GLU:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:9101:G4P:H5"	8:N:9101:G4P:C8	2.15	0.76
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.68	0.76
2:C:495:THR:HG23	2:C:517:ARG:HE	1.50	0.76
3:D:1376:MET:HE3	3:D:1421:LEU:HB2	1.67	0.76
3:N:41:ARG:HB2	9:N:2916:HOH:O	1.86	0.76
3:D:1197:ARG:HD2	3:D:1396:GLU:HB2	1.68	0.76
2:C:627:ARG:H	2:C:627:ARG:NE	1.83	0.76
1:K:58:ILE:HB	1:K:61:VAL:HB	1.67	0.76
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.67	0.75
1:L:76:VAL:HB	3:N:872:ARG:HH22	1.51	0.75
3:N:1194:CYS:HA	9:N:9487:HOH:O	1.86	0.75
1:K:214:ALA:HA	1:K:217:ILE:HD12	1.68	0.75
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.66	0.75
2:M:598:GLU:O	2:M:651:LYS:HG3	1.86	0.75
2:M:1005:MET:HG3	3:N:629:SER:HB2	1.68	0.75
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.66	0.75
1:A:67:THR:HA	9:A:9794:HOH:O	1.86	0.75
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.69	0.75
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.86	0.75
2:M:100:LEU:HD21	2:M:368:THR:HA	1.67	0.75
5:P:416:ARG:HD2	5:P:419:ARG:HB2	1.67	0.75
1:B:13:VAL:HA	9:B:9669:HOH:O	1.86	0.75
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.69	0.75
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.67	0.75
9:N:9282:HOH:O	4:O:17:TYR:HB3	1.86	0.75
2:M:571:LEU:HD23	2:M:700:TYR:HA	1.68	0.75
3:D:699:VAL:HG22	3:D:756:GLN:HE22	1.50	0.75
2:M:442:GLU:HB3	9:M:9245:HOH:O	1.87	0.75
2:C:89:THR:HA	2:C:129:ILE:O	1.86	0.75
3:D:1137:ARG:H	3:D:1137:ARG:HD2	1.52	0.75
2:M:786:LYS:HD2	9:M:9396:HOH:O	1.85	0.75
4:E:28:GLN:HB3	9:E:9553:HOH:O	1.87	0.75
2:M:724:ARG:HB2	2:M:740:GLU:HA	1.69	0.75
3:D:868:TYR:HD1	3:D:869:MET:H	1.31	0.75
3:N:794:GLN:NE2	3:N:795:VAL:H	1.85	0.75
2:M:1013:TYR:HE2	5:P:341:PRO:HD2	1.51	0.75
2:C:500:ASN:HA	9:C:9718:HOH:O	1.86	0.75
3:N:1217:ILE:H	3:N:1217:ILE:HD12	1.50	0.75
1:L:27:PRO:HG2	1:L:186:LEU:HD12	1.68	0.75
2:M:338:GLU:HA	2:M:341:THR:HG22	1.68	0.74
2:M:711:GLU:HG2	2:M:822:VAL:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:133:ILE:HD13	3:N:454:ALA:HB1	1.69	0.74
2:C:181:VAL:HB	9:C:9674:HOH:O	1.86	0.74
2:M:838:LYS:HG3	2:M:997:LEU:HB2	1.70	0.74
2:C:737:LEU:HB3	9:C:9568:HOH:O	1.86	0.74
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.67	0.74
2:M:324:ASP:HB3	2:M:327:HIS:HD2	1.51	0.74
5:P:393:THR:HG22	5:P:394:ARG:H	1.51	0.74
3:D:99:ALA:HA	3:D:575:GLN:HE22	1.52	0.74
2:M:965:GLU:HA	2:M:968:LEU:HD12	1.69	0.74
3:N:152:LEU:HD23	3:N:152:LEU:H	1.51	0.74
2:C:1016:ILE:HD12	5:F:317:LEU:HD21	1.67	0.74
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.70	0.74
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.68	0.74
1:K:56:VAL:HG13	1:K:142:VAL:HG12	1.70	0.74
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.02	0.74
5:F:393:THR:HG22	5:F:394:ARG:H	1.52	0.74
2:C:753:ASP:HA	9:D:9567:HOH:O	1.88	0.74
1:A:58:ILE:HB	1:A:61:VAL:HB	1.69	0.74
3:D:658:LEU:HA	3:D:661:MET:HE3	1.70	0.74
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.69	0.74
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.70	0.74
2:M:328:LEU:HD12	9:M:9297:HOH:O	1.87	0.74
2:M:585:GLU:HB2	9:M:9626:HOH:O	1.88	0.74
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.68	0.74
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.70	0.74
2:M:734:LEU:HD13	2:M:737:LEU:HD13	1.69	0.74
3:N:1402:ALA:HB1	9:N:9626:HOH:O	1.88	0.73
3:N:1382:THR:HG21	3:N:1418:LYS:HE3	1.70	0.73
3:N:191:LEU:HD13	3:N:195:VAL:HG11	1.70	0.73
3:D:756:GLN:HE21	3:D:760:ARG:HD2	1.51	0.73
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.68	0.73
3:N:1116:ASN:ND2	3:N:1193:THR:HB	2.03	0.73
9:C:9690:HOH:O	3:D:1064:GLY:HA2	1.87	0.73
3:N:890:VAL:HA	9:N:9430:HOH:O	1.88	0.73
2:C:724:ARG:HB2	2:C:740:GLU:HA	1.68	0.73
3:N:455:ARG:HH22	5:P:140:ARG:HB3	1.53	0.73
2:M:580:MET:HB2	9:M:9244:HOH:O	1.87	0.73
2:C:948:GLU:HA	9:C:2299:HOH:O	1.87	0.73
2:M:336:VAL:HA	2:M:339:LEU:HD12	1.68	0.73
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.69	0.73
2:M:546:LEU:HD12	2:M:565:GLN:NE2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1058:ASP:OD2	2:C:1083:GLU:HB2	1.88	0.73
2:M:325:ILE:HB	9:M:9421:HOH:O	1.88	0.73
2:M:89:THR:HA	2:M:129:ILE:O	1.88	0.73
3:D:534:ARG:HA	9:F:2094:HOH:O	1.88	0.73
2:M:395:LYS:HG2	2:M:397:GLU:HG2	1.71	0.73
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.51	0.73
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.71	0.73
2:M:568:ALA:HB1	2:M:668:LEU:HB3	1.69	0.73
3:N:441:ARG:HB3	3:N:443:VAL:HG23	1.69	0.73
3:D:1252:ILE:HG22	3:D:1253:THR:H	1.53	0.73
2:M:968:LEU:HB3	9:M:9311:HOH:O	1.88	0.73
2:M:94:LEU:HA	9:M:9263:HOH:O	1.86	0.73
5:F:164:LYS:HA	5:F:171:LYS:HZ3	1.54	0.73
3:N:52:PRO:HG2	9:N:9465:HOH:O	1.88	0.73
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.52	0.73
5:P:287:THR:HG23	5:P:289:GLU:HB2	1.70	0.73
3:D:1496:GLU:HG3	3:D:1500:LYS:HE3	1.71	0.73
1:L:120:VAL:HG23	9:L:3068:HOH:O	1.89	0.73
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.71	0.73
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.71	0.73
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.69	0.73
3:N:195:VAL:HB	3:N:205:TYR:HB2	1.69	0.73
2:M:492:ASP:HA	2:M:518:LYS:HB3	1.70	0.73
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.53	0.73
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.71	0.72
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.71	0.72
4:O:8:LYS:HG3	9:O:1143:HOH:O	1.89	0.72
3:D:675:ARG:O	3:D:678:GLU:HG2	1.88	0.72
2:C:118:ILE:H	2:C:118:ILE:HD13	1.53	0.72
1:A:214:ALA:HA	1:A:217:ILE:HD12	1.68	0.72
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.71	0.72
1:A:166:PRO:HB3	9:A:9709:HOH:O	1.89	0.72
3:D:534:ARG:HH21	5:F:315:VAL:HG21	1.54	0.72
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.71	0.72
2:M:176:VAL:HG22	2:M:182:VAL:HG13	1.70	0.72
1:L:89:PHE:HB3	1:L:94:LEU:HD13	1.71	0.72
2:C:1102:LEU:HB3	9:C:9776:HOH:O	1.89	0.72
3:N:1310:ARG:HE	3:N:1327:ARG:HB3	1.53	0.72
3:N:1314:LYS:HZ1	3:N:1317:ASP:HB2	1.54	0.72
4:O:87:LYS:HE2	4:O:91:ARG:HH21	1.53	0.72
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.71	0.72
3:D:1378:TYR:O	3:D:1420:LEU:HB3	1.90	0.72
3:D:1063:GLU:HG2	3:D:1064:GLY:H	1.54	0.72
3:N:1166:LEU:HD23	3:N:1166:LEU:H	1.54	0.72
1:L:204:SER:HA	9:L:2931:HOH:O	1.89	0.72
3:D:1254:GLN:HB2	9:D:2152:HOH:O	1.88	0.72
3:N:1118:ILE:HD11	3:N:1346:ARG:HE	1.53	0.72
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.70	0.72
3:D:31:THR:HA	9:D:9962:HOH:O	1.88	0.72
5:F:273:ARG:HA	5:F:276:ARG:HH11	1.54	0.72
2:C:1013:TYR:HB2	5:F:335:ASP:OD2	1.90	0.72
3:D:838:ARG:HH12	3:D:863:VAL:HG12	1.53	0.72
5:F:416:ARG:HD2	5:F:419:ARG:HB2	1.71	0.72
1:B:23:PHE:HA	9:B:9669:HOH:O	1.89	0.72
3:N:1495:ILE:HA	9:N:9438:HOH:O	1.87	0.72
3:D:54:LYS:HD3	3:D:55:ASP:H	1.54	0.72
3:N:1314:LYS:NZ	3:N:1317:ASP:HB2	2.04	0.72
1:L:225:PHE:HA	9:L:2122:HOH:O	1.90	0.72
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.72	0.72
3:D:834:THR:OG1	3:D:838:ARG:HB3	1.89	0.72
3:D:615:ARG:O	3:D:619:LEU:HB2	1.90	0.72
2:M:324:ASP:HA	9:M:2460:HOH:O	1.90	0.71
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.69	0.71
3:D:601:ARG:HH12	3:D:613:ARG:HH21	1.38	0.71
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.06	0.71
3:N:692:GLU:HG2	3:N:720:LEU:HD12	1.71	0.71
2:C:689:VAL:CG2	2:C:870:ILE:HB	2.20	0.71
2:C:777:ILE:HG12	9:C:2212:HOH:O	1.89	0.71
2:M:144:PRO:HA	2:M:163:ILE:HG23	1.73	0.71
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.55	0.71
1:K:94:LEU:HD21	1:K:119:ASP:HB2	1.71	0.71
1:B:123:MET:HG2	9:B:9676:HOH:O	1.90	0.71
1:K:117:VAL:HG22	9:K:4167:HOH:O	1.88	0.71
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.72	0.71
5:P:131:VAL:HG13	5:P:178:ARG:HG2	1.72	0.71
3:N:162:ARG:HA	3:N:449:SER:HB3	1.71	0.71
3:N:1330:ILE:HA	9:N:9632:HOH:O	1.90	0.71
2:C:371:LYS:O	2:C:372:LEU:HD12	1.91	0.71
3:D:1346:ARG:HA	3:D:1346:ARG:HE	1.54	0.71
3:N:1127:GLU:HB3	9:N:9298:HOH:O	1.90	0.71
1:L:176:ARG:HH12	3:N:884:ARG:NE	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:309:LYS:HA	5:F:312:GLN:OE1	1.91	0.71
2:M:1115:LEU:HD23	3:N:85:VAL:HA	1.73	0.71
2:M:584:GLU:HG2	9:M:9244:HOH:O	1.90	0.71
2:M:218:VAL:HG22	2:M:221:LEU:HD23	1.71	0.71
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.72	0.71
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.54	0.71
2:C:536:PRO:HD2	2:C:537:LYS:NZ	2.06	0.71
1:L:167:VAL:HG22	9:L:2964:HOH:O	1.90	0.71
2:M:184:MET:HG3	2:M:193:LEU:HD23	1.72	0.71
3:N:810:GLU:O	3:N:813:LEU:HG	1.91	0.71
3:N:827:ILE:HA	9:N:9636:HOH:O	1.89	0.71
3:N:662:GLU:HB2	9:N:9379:HOH:O	1.89	0.71
2:M:882:LEU:HD12	3:N:1061:PHE:HB3	1.73	0.71
2:M:621:VAL:HB	9:M:9858:HOH:O	1.91	0.71
2:M:468:ARG:HB3	9:M:9590:HOH:O	1.90	0.71
3:D:486:ARG:HH21	3:D:489:ARG:NE	1.88	0.70
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.73	0.70
2:C:259:GLY:HA3	9:C:2199:HOH:O	1.91	0.70
1:A:158:ILE:HG12	9:A:9709:HOH:O	1.90	0.70
2:M:101:ILE:HG22	2:M:102:HIS:H	1.56	0.70
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.71	0.70
1:L:41:ARG:HH11	1:L:177:VAL:HB	1.56	0.70
2:C:889:HIS:HE1	3:D:951:ILE:H	1.38	0.70
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.71	0.70
2:C:957:LYS:HB3	9:C:9884:HOH:O	1.90	0.70
2:M:176:VAL:HG13	2:M:182:VAL:HG22	1.73	0.70
3:N:64:LYS:HB2	5:P:376:ILE:O	1.91	0.70
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.73	0.70
3:D:1432:LYS:CD	3:D:1433:SER:H	2.01	0.70
3:D:1462:LEU:HD23	9:D:3112:HOH:O	1.89	0.70
2:C:874:LEU:HB2	9:C:2136:HOH:O	1.91	0.70
2:M:290:LEU:HD12	2:M:302:VAL:HG11	1.72	0.70
2:C:86:LYS:HG3	2:C:813:VAL:HG12	1.72	0.70
2:M:413:LEU:H	2:M:413:LEU:HD12	1.56	0.70
3:N:507:ASN:HA	9:N:9943:HOH:O	1.91	0.70
2:C:336:VAL:HB	9:C:9899:HOH:O	1.91	0.70
3:N:1373:ARG:HG2	3:N:1374:GLN:NE2	2.06	0.70
2:C:285:LEU:HD21	2:C:289:THR:HA	1.73	0.70
3:N:1410:GLU:HA	9:N:9265:HOH:O	1.91	0.70
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	1.74	0.70
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:ILE:HD12	9:C:9856:HOH:O	1.91	0.70
2:C:385:PHE:O	2:C:389:SER:HB3	1.91	0.70
3:D:815:ALA:HB3	9:D:9733:HOH:O	1.92	0.70
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.73	0.70
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.74	0.70
1:A:146:ARG:HG2	9:A:9574:HOH:O	1.91	0.70
2:C:473:ARG:HE	2:C:531:PHE:HE1	1.39	0.70
1:B:133:GLU:HG3	1:B:134:GLU:H	1.56	0.70
3:N:709:HIS:HA	3:N:1227:GLN:HG2	1.73	0.70
1:K:91:ASN:HA	9:K:1224:HOH:O	1.91	0.70
5:P:184:ARG:HG2	5:P:188:ILE:HD11	1.74	0.70
2:M:1119:ARG:HE	2:M:1119:ARG:HA	1.57	0.70
3:D:119:SER:CB	3:D:123:LEU:HB2	2.22	0.70
2:M:130:ASN:HA	9:M:2315:HOH:O	1.91	0.70
4:E:32:ARG:HD3	9:E:9553:HOH:O	1.91	0.70
2:C:861:LEU:HD23	2:C:863:ASP:H	1.57	0.70
2:M:707:ARG:HD2	9:M:9630:HOH:O	1.91	0.70
2:C:405:ARG:NH1	2:C:409:ARG:HH21	1.90	0.70
2:C:689:VAL:HG23	2:C:870:ILE:HB	1.73	0.70
1:L:151:VAL:HB	1:L:169:ALA:HB3	1.74	0.70
1:A:219:ARG:HH12	1:B:219:ARG:HG2	1.57	0.70
3:N:131:LYS:HA	3:N:456:MET:HG3	1.72	0.70
5:F:135:ILE:HD11	5:F:178:ARG:HD2	1.73	0.70
2:M:288:ARG:HG3	2:M:288:ARG:HH11	1.55	0.69
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.07	0.69
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.06	0.69
2:M:776:SER:HA	2:M:780:GLU:HB3	1.73	0.69
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.72	0.69
1:B:80:LEU:HG	3:D:844:ALA:HB2	1.72	0.69
3:D:710:ARG:HG2	3:D:710:ARG:HH11	1.56	0.69
2:C:197:LEU:HD13	2:C:207:LEU:HD21	1.74	0.69
5:F:270:LYS:HB3	5:F:295:MET:SD	2.31	0.69
1:L:62:LEU:HD12	9:L:6647:HOH:O	1.91	0.69
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.72	0.69
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.73	0.69
2:M:412:ALA:HA	9:M:9312:HOH:O	1.91	0.69
3:N:1157:GLY:HA3	9:N:9424:HOH:O	1.92	0.69
1:A:22:GLU:HB3	9:A:9573:HOH:O	1.92	0.69
2:M:777:ILE:O	5:P:409:LYS:HD2	1.92	0.69
2:M:284:ARG:HG2	2:M:285:LEU:H	1.54	0.69
3:D:537:THR:HG22	9:F:9559:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:39:ARG:NE	2:M:39:ARG:HA	2.07	0.69
2:C:776:SER:HA	2:C:780:GLU:HB3	1.72	0.69
2:C:969:GLN:HB3	9:C:9615:HOH:O	1.91	0.69
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.73	0.69
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.73	0.69
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.75	0.69
4:E:40:LEU:HD13	4:E:45:ARG:HD2	1.74	0.69
3:N:711:LEU:HD11	9:N:9759:HOH:O	1.92	0.69
3:D:119:SER:H	3:D:123:LEU:HD13	1.56	0.69
2:C:430:VAL:CG1	3:D:1075:HIS:HA	2.23	0.69
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.73	0.69
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.74	0.69
5:F:366:ALA:HB2	9:F:2032:HOH:O	1.91	0.69
2:C:710:ILE:HD11	2:C:758:ARG:NE	2.07	0.69
2:C:557:ARG:NH1	2:C:879:ARG:HE	1.90	0.69
3:D:838:ARG:HA	9:D:9613:HOH:O	1.92	0.69
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.73	0.69
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.57	0.69
2:M:803:THR:HG22	2:M:825:VAL:HG13	1.75	0.69
3:D:156:GLU:HB2	9:D:3232:HOH:O	1.93	0.69
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.75	0.69
2:M:979:THR:HG23	2:M:981:GLU:H	1.55	0.69
2:C:436:GLY:HA2	2:C:538:GLN:O	1.92	0.69
1:L:112:ARG:HD2	9:L:1944:HOH:O	1.92	0.69
5:P:337:HIS:HA	9:P:2159:HOH:O	1.92	0.69
3:D:994:GLN:HB2	9:D:2834:HOH:O	1.93	0.69
2:M:336:VAL:HG21	9:M:9234:HOH:O	1.93	0.69
2:C:102:HIS:HE1	2:C:367:LEU:HD21	1.56	0.69
2:M:436:GLY:HA2	2:M:538:GLN:O	1.93	0.69
3:D:549:ASN:HB3	9:D:2045:HOH:O	1.92	0.69
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.56	0.69
3:N:192:ALA:O	3:N:195:VAL:HG23	1.93	0.69
3:N:127:LEU:HD21	3:N:461:ILE:HD11	1.74	0.69
2:M:89:THR:O	2:M:91:GLN:HG3	1.93	0.69
3:N:447:VAL:HG11	9:N:2028:HOH:O	1.93	0.69
2:C:1052:MET:HE3	2:C:1056:LYS:HD3	1.74	0.69
4:O:70:THR:HG22	9:O:1901:HOH:O	1.93	0.69
4:E:51:LEU:HG	4:E:53:GLY:H	1.58	0.69
3:D:116:LEU:HB3	3:D:118:LEU:HD13	1.73	0.69
3:D:179:VAL:HG22	3:D:389:GLU:HG3	1.75	0.69
5:F:388:ALA:HB3	9:F:9936:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.57	0.69
1:K:86:VAL:HG12	1:K:124:ASN:ND2	2.08	0.69
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.75	0.69
2:M:3:ILE:HG21	9:M:2484:HOH:O	1.93	0.69
1:A:53:VAL:HG12	1:A:167:VAL:HG21	1.72	0.69
2:M:328:LEU:HD13	2:M:433:THR:OG1	1.92	0.68
3:N:119:SER:OG	3:N:123:LEU:HD13	1.94	0.68
3:N:194:GLY:HA2	3:N:206:ARG:HD2	1.76	0.68
3:N:1118:ILE:HD11	3:N:1346:ARG:NE	2.08	0.68
3:D:798:GLU:HG2	3:D:799:LYS:H	1.57	0.68
3:D:162:ARG:NH2	3:D:434:ARG:HH21	1.90	0.68
3:D:194:GLY:HA2	3:D:206:ARG:HD2	1.74	0.68
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.75	0.68
3:N:216:VAL:HA	9:N:2353:HOH:O	1.91	0.68
1:A:117:VAL:HG12	9:A:9774:HOH:O	1.94	0.68
3:N:477:LEU:HD21	3:N:495:ARG:HE	1.56	0.68
2:M:511:GLU:O	2:M:526:PRO:HD3	1.94	0.68
2:C:237:ARG:HG2	9:C:2116:HOH:O	1.94	0.68
5:F:76:SER:HB3	9:F:9637:HOH:O	1.92	0.68
3:N:1239:ARG:HB2	9:N:2464:HOH:O	1.92	0.68
2:C:751:PRO:HB2	3:D:680:GLN:HG3	1.74	0.68
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.08	0.68
3:N:141:ILE:H	3:N:141:ILE:HD12	1.58	0.68
3:N:161:LEU:HD21	3:N:452:ILE:HD13	1.75	0.68
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.75	0.68
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.76	0.68
3:D:411:THR:HG21	9:D:9778:HOH:O	1.94	0.68
3:N:796:ARG:HH21	3:N:828:LYS:HE2	1.58	0.68
3:D:73:CYS:HB3	3:D:76:CYS:O	1.93	0.68
3:N:1435:LEU:HG	3:N:1467:ILE:HD12	1.76	0.68
3:D:173:PRO:HD3	3:D:178:LEU:HD12	1.75	0.68
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.75	0.68
2:C:1014:SER:HB3	9:C:9664:HOH:O	1.92	0.68
1:K:86:VAL:HG12	1:K:124:ASN:HD22	1.59	0.68
3:D:1077:ALA:HB2	9:D:9673:HOH:O	1.93	0.68
3:D:935:LYS:HZ2	3:D:935:LYS:HB3	1.57	0.68
2:C:492:ASP:HA	2:C:518:LYS:HB3	1.74	0.68
5:P:273:ARG:HG3	9:P:1952:HOH:O	1.93	0.68
2:C:577:PRO:HA	2:C:671:ASN:ND2	2.02	0.68
3:N:119:SER:HB3	9:N:9548:HOH:O	1.94	0.68
2:C:24:GLU:HB3	2:C:28:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1277:ILE:HD12	9:N:9684:HOH:O	1.94	0.68
3:D:876:SER:O	3:D:880:ILE:HG12	1.93	0.68
3:D:914:LEU:HA	9:D:2987:HOH:O	1.94	0.68
3:D:804:LEU:HD21	3:D:829:VAL:HG21	1.76	0.68
3:D:481:MET:HG3	3:D:493:ARG:HG2	1.75	0.68
2:M:164:PRO:CA	2:M:266:ARG:HH22	2.07	0.68
3:D:976:GLN:HA	9:D:9904:HOH:O	1.94	0.68
2:C:952:LEU:HD12	2:C:969:GLN:NE2	2.07	0.68
1:B:208:LEU:HD23	9:B:9568:HOH:O	1.94	0.68
4:O:70:THR:HG21	9:O:2018:HOH:O	1.94	0.68
3:D:1401:GLU:HB3	9:D:9816:HOH:O	1.93	0.68
2:C:760:SER:O	2:C:785:VAL:HG22	1.94	0.68
9:K:5477:HOH:O	2:M:605:LYS:HA	1.93	0.68
1:K:71:VAL:HA	9:K:1208:HOH:O	1.93	0.68
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.76	0.67
2:M:284:ARG:HG2	2:M:285:LEU:N	2.09	0.67
5:P:132:ARG:O	5:P:136:LEU:HG	1.94	0.67
2:C:358:ARG:HH21	2:C:373:VAL:N	1.91	0.67
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.75	0.67
2:C:12:VAL:HG22	2:C:13:ILE:HG23	1.76	0.67
3:D:785:ILE:HG12	3:D:935:LYS:HA	1.73	0.67
5:F:77:THR:O	5:F:81:VAL:HG23	1.94	0.67
3:D:730:PRO:HA	3:D:733:CYS:SG	2.35	0.67
5:P:373:LYS:HG2	9:P:2070:HOH:O	1.94	0.67
3:D:629:SER:HB3	3:D:726:ILE:HD11	1.77	0.67
3:D:68:PHE:HB3	9:D:9610:HOH:O	1.94	0.67
3:N:399:ARG:HG3	9:N:2124:HOH:O	1.94	0.67
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.75	0.67
3:D:488:ARG:NE	3:D:488:ARG:H	1.92	0.67
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.76	0.67
3:N:167:GLU:HA	9:N:9499:HOH:O	1.95	0.67
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.94	0.67
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.77	0.67
5:P:163:LEU:HD22	5:P:174:LEU:HG	1.77	0.67
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.75	0.67
3:N:1121:PRO:HD3	3:N:1346:ARG:NH2	2.09	0.67
2:M:183:SER:HB3	2:M:190:LYS:HD3	1.76	0.67
1:B:41:ARG:HH11	1:B:177:VAL:HB	1.58	0.67
2:C:31:GLN:NE2	2:C:40:GLU:HB2	2.09	0.67
2:M:716:LYS:HA	2:M:716:LYS:HE3	1.75	0.67
2:C:54:ILE:HG21	9:C:2671:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1049:LEU:HD22	3:D:1472:ILE:HD11	1.77	0.67
3:N:481:MET:HE1	3:N:493:ARG:HE	1.60	0.67
2:M:52:PHE:HB3	9:M:9629:HOH:O	1.95	0.67
3:D:1131:SER:O	3:D:1133:ARG:HG3	1.95	0.67
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.77	0.67
2:M:339:LEU:HG	9:M:9771:HOH:O	1.95	0.67
2:M:50:GLU:HG2	2:M:265:ARG:NH1	2.09	0.67
2:C:841:ASN:HD21	2:C:845:ASN:N	1.93	0.67
2:C:23:VAL:HG12	9:C:2056:HOH:O	1.95	0.67
2:M:1005:MET:HE3	3:N:645:PRO:HG2	1.75	0.67
2:C:1019:GLN:HG2	9:C:9664:HOH:O	1.95	0.67
2:C:266:ARG:HD3	2:C:288:ARG:HE	1.57	0.67
1:K:222:LEU:HD12	1:L:215:VAL:HB	1.75	0.67
3:D:1395:LEU:HB2	9:D:2424:HOH:O	1.93	0.67
3:D:576:GLU:HG3	9:F:9597:HOH:O	1.94	0.67
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.75	0.67
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.77	0.67
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.75	0.67
5:F:234:LYS:HD3	5:F:236:SER:HB2	1.77	0.67
3:N:1381:VAL:HG23	9:N:9527:HOH:O	1.95	0.67
1:L:132:LEU:HB3	9:L:1114:HOH:O	1.95	0.67
2:M:64:LEU:HD22	2:M:359:MET:HG3	1.76	0.67
2:M:266:ARG:HD3	2:M:288:ARG:NH1	2.10	0.67
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.77	0.67
1:L:77:GLU:HB3	9:L:1341:HOH:O	1.95	0.67
1:A:66:SER:HA	9:A:9605:HOH:O	1.94	0.67
1:K:12:THR:HG23	1:K:24:VAL:HB	1.76	0.67
2:M:269:LEU:HA	2:M:288:ARG:HD2	1.77	0.67
1:B:132:LEU:HB3	9:B:9733:HOH:O	1.94	0.67
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.76	0.67
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.76	0.67
1:A:41:ARG:HH11	1:A:177:VAL:HB	1.59	0.67
3:N:1336:LEU:HD22	3:N:1421:LEU:HB2	1.77	0.67
3:N:699:VAL:H	3:N:756:GLN:NE2	1.93	0.67
1:A:11:PHE:HB2	9:A:9706:HOH:O	1.94	0.67
2:C:300:ASP:OD2	2:C:303:PHE:HB2	1.94	0.67
3:D:28:LYS:HD2	3:D:41:ARG:HD2	1.76	0.67
2:M:1090:LYS:HE2	3:N:88:TYR:O	1.95	0.67
1:K:102:LYS:HG3	9:K:2209:HOH:O	1.95	0.67
5:P:102:LEU:O	5:P:106:VAL:HG23	1.95	0.67
5:P:358:LEU:HD11	5:P:370:LYS:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:ARG:HD3	2:C:543:ASN:CG	2.16	0.66
2:M:841:ASN:HD21	2:M:845:ASN:N	1.93	0.66
2:M:397:GLU:HG3	2:M:633:GLN:HE22	1.60	0.66
3:N:1313:VAL:HA	9:N:9426:HOH:O	1.94	0.66
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.10	0.66
2:C:267:TYR:HE1	2:C:338:GLU:HG3	1.60	0.66
2:M:489:THR:HA	9:M:9368:HOH:O	1.94	0.66
1:B:9:PRO:HB3	1:B:25:LEU:HG	1.77	0.66
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.25	0.66
2:M:490:GLU:HG2	2:M:494:TYR:HE1	1.59	0.66
3:N:1301:LYS:HG2	9:N:2064:HOH:O	1.96	0.66
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.76	0.66
1:L:26:GLU:HB3	1:L:194:LYS:HG3	1.76	0.66
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.77	0.66
2:M:759:THR:HB	2:M:785:VAL:HG11	1.77	0.66
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.60	0.66
2:M:16:PRO:HB2	2:M:460:ARG:HD3	1.78	0.66
3:N:197:SER:HB2	3:N:205:TYR:CE1	2.30	0.66
3:D:178:LEU:HG	3:D:200:ASP:H	1.61	0.66
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.59	0.66
1:A:2:LEU:HA	1:A:6:LEU:HD22	1.77	0.66
1:K:97:VAL:HG23	9:K:1044:HOH:O	1.95	0.66
1:B:46:SER:O	1:B:148:VAL:HB	1.95	0.66
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.77	0.66
3:D:168:THR:HB	3:D:393:ILE:HD12	1.78	0.66
3:N:481:MET:CE	3:N:493:ARG:HE	2.08	0.66
1:L:186:LEU:HB2	9:L:1608:HOH:O	1.96	0.66
4:E:46:PRO:HD3	4:E:66:LYS:HG2	1.77	0.66
2:C:527:GLU:HG3	9:C:2408:HOH:O	1.95	0.66
3:N:537:THR:C	5:P:317:LEU:HB2	2.15	0.66
3:D:1314:LYS:HG2	9:D:2456:HOH:O	1.94	0.66
1:A:185:ARG:HD2	9:A:9581:HOH:O	1.95	0.66
3:N:95:LEU:HD12	3:N:515:GLU:HA	1.77	0.66
2:C:130:ASN:HA	9:C:9898:HOH:O	1.94	0.66
3:N:825:ALA:HB1	9:N:9618:HOH:O	1.95	0.66
2:C:783:ARG:HG2	2:C:785:VAL:HB	1.78	0.66
5:F:128:ARG:HD2	9:F:9581:HOH:O	1.96	0.66
3:N:1242:HIS:CE1	3:N:1266:ARG:HH11	2.13	0.66
5:P:302:LYS:HB3	9:P:3098:HOH:O	1.95	0.66
2:M:162:ILE:HD12	2:M:172:ILE:HB	1.77	0.66
3:D:684:LYS:HE2	9:D:9654:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.76	0.66
5:P:140:ARG:HG3	9:P:2295:HOH:O	1.95	0.66
2:C:780:GLU:HG3	2:C:781:LYS:H	1.61	0.66
1:B:137:ARG:HH12	1:B:139:ASN:HB3	1.61	0.66
3:N:899:LEU:HD23	3:N:917:GLN:HB3	1.78	0.66
9:D:2753:HOH:O	5:F:171:LYS:HG2	1.94	0.66
3:D:97:THR:HG22	9:D:9686:HOH:O	1.96	0.66
2:C:250:ARG:NH2	2:C:254:VAL:HB	2.11	0.66
5:P:158:GLU:HA	5:P:161:GLN:HE21	1.61	0.66
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.61	0.66
2:M:129:ILE:HD13	9:M:9309:HOH:O	1.94	0.66
3:D:1265:ALA:HB1	9:D:9823:HOH:O	1.96	0.66
2:C:338:GLU:HA	2:C:341:THR:HG22	1.77	0.66
3:N:39:PRO:HB3	3:N:45:PHE:O	1.95	0.66
3:N:1196:THR:HA	9:N:9588:HOH:O	1.96	0.66
3:N:1501:GLU:HB3	9:N:9522:HOH:O	1.96	0.66
5:P:170:HIS:HA	5:P:173:TYR:HD1	1.61	0.66
2:C:66:LEU:HD13	2:C:100:LEU:HB3	1.78	0.66
2:M:394:PHE:HA	9:M:9211:HOH:O	1.96	0.66
3:N:984:THR:H	3:N:987:GLU:CD	1.99	0.66
2:C:176:VAL:HG12	2:C:182:VAL:HG22	1.77	0.66
5:F:155:THR:HA	9:F:9647:HOH:O	1.96	0.65
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.43	0.65
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.26	0.65
2:M:905:ILE:HG12	9:M:9307:HOH:O	1.96	0.65
2:M:73:LEU:HB3	9:M:9468:HOH:O	1.97	0.65
1:A:102:LYS:HG2	9:A:9611:HOH:O	1.95	0.65
2:C:814:GLU:HG3	9:C:9712:HOH:O	1.95	0.65
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.59	0.65
2:M:451:LEU:HA	9:M:9532:HOH:O	1.97	0.65
2:M:829:GLN:NE2	2:M:831:ARG:HD3	2.06	0.65
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.22	0.65
3:D:475:LYS:HD3	3:D:478:LEU:HD12	1.79	0.65
2:M:230:ARG:NE	2:M:237:ARG:HH22	1.94	0.65
5:P:150:THR:HG23	5:P:155:THR:HG21	1.79	0.65
2:C:336:VAL:HG12	9:C:2001:HOH:O	1.96	0.65
2:C:534:VAL:H	2:C:538:GLN:HE22	1.44	0.65
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.62	0.65
2:M:744:ARG:HG3	2:M:747:ALA:HB2	1.77	0.65
1:B:39:PRO:O	1:B:43:ILE:HG12	1.95	0.65
3:D:646:LYS:HA	3:D:720:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:ILE:HG12	9:C:9584:HOH:O	1.95	0.65
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.61	0.65
1:A:50:GLY:HA3	1:A:173:PRO:HG3	1.78	0.65
4:E:88:GLU:HA	9:E:9574:HOH:O	1.95	0.65
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.76	0.65
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.78	0.65
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.79	0.65
2:M:338:GLU:HB3	9:M:9771:HOH:O	1.96	0.65
2:C:1115:LEU:H	2:C:1115:LEU:HD12	1.62	0.65
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.79	0.65
2:M:282:GLY:HA2	2:M:308:ARG:HH21	1.61	0.65
4:E:25:LYS:HA	4:E:28:GLN:CD	2.16	0.65
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.78	0.65
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.62	0.65
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.79	0.65
2:M:21:ILE:HD12	2:M:21:ILE:H	1.61	0.65
1:B:44:LEU:HD23	1:B:48:ILE:HD11	1.77	0.65
3:N:212:ARG:HA	9:N:9240:HOH:O	1.96	0.65
3:N:9:ARG:HD3	3:N:1456:LYS:HG2	1.79	0.65
3:N:175:VAL:HG13	3:N:217:LYS:CB	2.27	0.65
3:N:781:PRO:HG2	3:N:911:LEU:HD23	1.79	0.65
1:A:59:GLU:HG3	1:A:60:ASP:H	1.61	0.65
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.59	0.65
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.10	0.65
1:K:57:TYR:HE1	1:K:163:ASN:HB2	1.62	0.65
3:N:128:TYR:HE2	3:N:458:ALA:HA	1.62	0.65
3:N:907:GLU:HA	9:N:9335:HOH:O	1.96	0.65
2:M:734:LEU:HA	2:M:737:LEU:HD13	1.79	0.65
3:D:998:GLU:HA	9:D:2729:HOH:O	1.97	0.65
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.78	0.65
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.78	0.65
3:N:11:ALA:HB1	3:N:507:ASN:OD1	1.97	0.65
1:K:221:HIS:HA	1:K:224:TYR:CE2	2.31	0.65
2:M:39:ARG:HE	2:M:39:ARG:HA	1.62	0.65
5:P:412:GLU:OE1	5:P:418:LEU:HD13	1.97	0.65
2:M:1040:LEU:HG	9:M:9264:HOH:O	1.97	0.65
3:D:1388:ARG:N	3:D:1388:ARG:HD2	2.08	0.65
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.11	0.65
3:N:1239:ARG:HA	9:N:9644:HOH:O	1.96	0.65
2:C:184:MET:HE3	2:C:186:VAL:HG13	1.79	0.65
2:M:875:GLY:HA3	9:M:9227:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:HG3	9:C:9673:HOH:O	1.96	0.65
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.77	0.65
1:L:75:VAL:HB	9:L:2024:HOH:O	1.97	0.65
3:N:1181:GLY:HA3	9:N:9860:HOH:O	1.95	0.65
3:N:1459:LEU:HD12	3:N:1470:ARG:NH1	2.12	0.65
5:P:261:PRO:HG3	9:P:4201:HOH:O	1.97	0.65
3:N:470:LEU:HD22	3:N:499:VAL:HG13	1.78	0.65
2:M:627:ARG:HG3	2:M:628:PHE:H	1.61	0.65
2:M:266:ARG:HG2	9:M:9612:HOH:O	1.95	0.65
3:N:52:PRO:HG3	3:N:80:VAL:HG23	1.78	0.65
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.37	0.65
3:D:1042:ARG:O	3:D:1057:VAL:HB	1.96	0.65
2:M:380:ALA:HB1	9:M:2219:HOH:O	1.97	0.65
2:C:103:LYS:HA	2:C:103:LYS:HE2	1.79	0.65
1:A:86:VAL:HG12	1:A:124:ASN:ND2	2.11	0.65
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.78	0.65
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.78	0.64
2:M:143:SER:HB2	2:M:276:LYS:HE2	1.79	0.64
3:N:484:PRO:O	3:N:489:ARG:HD2	1.97	0.64
3:N:800:LYS:HG3	3:N:830:ALA:HB3	1.79	0.64
1:A:206:THR:HG22	1:A:209:GLU:H	1.62	0.64
3:N:1310:ARG:NE	3:N:1327:ARG:HB3	2.13	0.64
3:D:162:ARG:HH22	3:D:434:ARG:HH21	1.43	0.64
3:N:126:VAL:HG13	3:N:132:TYR:HB2	1.79	0.64
2:M:17:PRO:HB2	2:M:20:GLU:HB2	1.77	0.64
3:N:984:THR:HG22	3:N:987:GLU:CG	2.27	0.64
5:P:130:VAL:HG13	5:P:156:VAL:HG23	1.78	0.64
2:C:759:THR:HG22	9:C:9784:HOH:O	1.98	0.64
1:K:64:GLU:HG3	1:K:165:ILE:HD12	1.79	0.64
3:D:440:VAL:HA	9:D:2195:HOH:O	1.97	0.64
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.78	0.64
2:C:580:MET:O	2:C:902:ILE:HA	1.98	0.64
3:N:1432:LYS:NZ	3:N:1460:ILE:HB	2.12	0.64
1:A:193:ASP:HA	9:C:9642:HOH:O	1.95	0.64
3:N:983:LEU:HB2	9:N:9836:HOH:O	1.96	0.64
1:K:72:LYS:NZ	2:M:644:VAL:HA	2.10	0.64
3:N:1034:GLN:HA	3:N:1037:GLN:HE21	1.63	0.64
2:M:232:GLU:HA	9:M:9931:HOH:O	1.98	0.64
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.79	0.64
2:C:946:ARG:HD2	2:C:984:GLU:HB2	1.77	0.64
1:B:100:LEU:HD12	1:B:115:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1189:ARG:HG2	9:D:9851:HOH:O	1.96	0.64
2:M:462:ASP:HB2	9:M:9913:HOH:O	1.97	0.64
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.62	0.64
2:M:1020:PRO:O	3:N:622:ARG:HD2	1.97	0.64
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.80	0.64
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.97	0.64
3:D:660:LYS:HA	3:D:663:GLU:HG3	1.79	0.64
3:N:601:ARG:HB2	5:P:318:GLU:OE1	1.97	0.64
2:C:1054:THR:HG21	2:C:1079:PRO:CB	2.20	0.64
5:F:286:PRO:HA	9:F:9596:HOH:O	1.97	0.64
3:N:984:THR:HG23	3:N:986:ARG:H	1.63	0.64
2:M:760:SER:HA	9:M:9228:HOH:O	1.97	0.64
1:A:88:ARG:HG3	1:A:204:SER:O	1.98	0.64
3:N:466:LYS:HD2	3:N:510:GLU:HG2	1.78	0.64
1:L:220:GLU:HG3	9:L:3319:HOH:O	1.96	0.64
3:N:71:LYS:N	3:N:71:LYS:HD2	2.12	0.64
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.62	0.64
1:K:48:ILE:HG22	1:K:173:PRO:HD2	1.79	0.64
3:N:794:GLN:HE21	3:N:795:VAL:N	1.95	0.64
2:M:1018:GLN:HG3	2:M:1060:ILE:HD11	1.78	0.64
3:D:806:PHE:O	3:D:808:THR:N	2.31	0.64
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.63	0.64
2:M:575:GLN:HB3	2:M:670:GLN:HA	1.80	0.64
2:C:739:GLU:HG2	9:C:9982:HOH:O	1.96	0.64
2:M:943:VAL:HG13	2:M:985:GLY:H	1.62	0.64
1:A:153:ALA:HA	1:A:156:HIS:NE2	2.12	0.64
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.80	0.64
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.12	0.64
2:C:606:VAL:HA	9:C:9584:HOH:O	1.95	0.64
3:D:513:ILE:HA	9:D:9584:HOH:O	1.96	0.64
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.80	0.64
2:C:831:ARG:NH2	2:C:999:HIS:HB2	2.12	0.64
3:N:65:ARG:HB2	5:P:375:LEU:CA	2.28	0.64
3:N:161:LEU:O	3:N:449:SER:HB2	1.98	0.64
2:M:159:ILE:HA	9:M:2059:HOH:O	1.96	0.64
3:D:873:LEU:HD12	3:D:873:LEU:H	1.63	0.64
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.64
3:N:64:LYS:NZ	5:P:377:ASP:HA	2.12	0.64
1:B:162:ILE:HG23	1:B:163:ASN:ND2	2.11	0.64
1:L:39:PRO:O	1:L:43:ILE:HG12	1.97	0.64
3:D:1503:VAL:HG12	9:D:9672:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:468:LEU:HB3	9:N:9474:HOH:O	1.98	0.64
3:D:1058:ARG:HG3	3:D:1058:ARG:HH11	1.63	0.64
2:C:1114:GLY:HA2	9:C:2283:HOH:O	1.96	0.64
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.79	0.64
2:C:403:SER:O	2:C:407:LYS:HD3	1.98	0.64
1:K:59:GLU:HG3	1:K:60:ASP:H	1.63	0.64
5:P:271:LEU:HD22	5:P:291:ILE:HD11	1.80	0.64
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.98	0.64
3:D:860:LEU:O	3:D:877:PRO:HD2	1.97	0.64
2:C:110:GLU:H	2:C:368:THR:HG21	1.63	0.64
2:C:17:PRO:HB2	2:C:20:GLU:HB2	1.80	0.64
2:M:721:ARG:NH2	2:M:783:ARG:HH21	1.96	0.64
1:L:100:LEU:HD12	1:L:115:LEU:HD21	1.80	0.64
3:N:925:GLU:HB3	9:O:6558:HOH:O	1.98	0.64
3:D:141:ILE:HD13	3:D:450:TYR:H	1.63	0.64
3:D:135:LEU:HD21	3:D:452:ILE:HG13	1.80	0.64
3:D:6:ARG:HH11	3:D:6:ARG:HB3	1.61	0.64
3:N:794:GLN:NE2	3:N:795:VAL:N	2.47	0.64
3:N:834:THR:HG22	3:N:838:ARG:HE	1.62	0.64
3:N:850:LEU:H	3:N:850:LEU:HD12	1.62	0.64
9:C:9880:HOH:O	3:D:656:PHE:HA	1.97	0.64
3:D:694:VAL:HA	9:D:2200:HOH:O	1.97	0.64
1:L:44:LEU:HD23	1:L:48:ILE:HD11	1.79	0.64
5:F:132:ARG:NH2	5:F:184:ARG:HH12	1.96	0.64
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.98	0.63
3:N:462:GLN:HG3	3:N:513:ILE:HD13	1.79	0.63
2:M:325:ILE:O	2:M:331:ARG:HG3	1.97	0.63
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.18	0.63
1:B:112:ARG:HD2	9:B:9726:HOH:O	1.97	0.63
2:C:133:ASP:HB2	2:C:632:ASN:HD21	1.62	0.63
2:C:139:GLN:HA	2:C:411:SER:O	1.97	0.63
5:P:184:ARG:O	5:P:188:ILE:HG13	1.99	0.63
3:D:690:ALA:HA	9:D:9783:HOH:O	1.97	0.63
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.78	0.63
3:D:149:LYS:HD3	3:D:149:LYS:H	1.61	0.63
3:D:12:LEU:HD11	3:D:512:MET:HG2	1.77	0.63
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.13	0.63
3:N:798:GLU:HG2	3:N:799:LYS:H	1.62	0.63
1:K:42:ARG:HA	9:K:1228:HOH:O	1.98	0.63
2:M:1059:ASP:HA	9:M:9233:HOH:O	1.98	0.63
2:M:1020:PRO:HD2	3:N:622:ARG:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:704:ARG:HG2	9:N:9545:HOH:O	1.98	0.63
1:K:25:LEU:HD11	9:L:4548:HOH:O	1.97	0.63
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.80	0.63
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.28	0.63
2:M:721:ARG:HG2	9:M:9669:HOH:O	1.98	0.63
2:M:84:ARG:NH1	2:M:128:ILE:HG12	2.13	0.63
2:C:47:ALA:HB3	9:C:9646:HOH:O	1.97	0.63
1:A:74:ASP:HA	9:A:9794:HOH:O	1.99	0.63
2:M:404:LEU:HD23	2:M:587:VAL:HG13	1.80	0.63
5:P:94:LEU:HD13	5:P:96:LEU:H	1.62	0.63
1:A:18:ARG:HD3	1:A:123:MET:HE3	1.81	0.63
1:A:39:PRO:O	1:A:43:ILE:HG12	1.98	0.63
2:C:823:VAL:HG13	9:C:9907:HOH:O	1.98	0.63
1:K:180:GLN:HB3	9:K:1076:HOH:O	1.97	0.63
1:A:73:GLU:HG2	9:A:9656:HOH:O	1.97	0.63
5:P:266:GLU:HB2	5:P:270:LYS:NZ	2.12	0.63
3:N:172:PRO:HD2	3:N:389:GLU:O	1.98	0.63
3:N:9:ARG:HH12	3:N:11:ALA:HB2	1.63	0.63
2:M:331:ARG:NH1	2:M:427:VAL:HG13	2.12	0.63
1:L:185:ARG:NH1	3:N:692:GLU:HG3	2.13	0.63
3:D:777:PRO:HB2	3:D:912:LYS:HD2	1.80	0.63
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.64	0.63
2:M:1016:ILE:HD12	3:N:526:PRO:HG2	1.80	0.63
3:N:429:SER:HG	3:N:432:TYR:HD2	1.46	0.63
2:M:1007:ALA:HB2	9:M:9335:HOH:O	1.98	0.63
2:M:493:ARG:HG3	9:M:9314:HOH:O	1.97	0.63
3:N:1432:LYS:HZ3	3:N:1460:ILE:HB	1.63	0.63
5:P:291:ILE:HD13	5:P:304:VAL:HG13	1.79	0.63
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.80	0.63
3:D:1269:LYS:HD2	9:D:2737:HOH:O	1.98	0.63
1:A:170:VAL:HG21	9:A:9702:HOH:O	1.98	0.63
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	1.98	0.63
2:M:164:PRO:HA	2:M:266:ARG:NH1	2.13	0.63
2:C:987:ILE:HG23	9:C:9757:HOH:O	1.98	0.63
3:N:1373:ARG:HG2	3:N:1374:GLN:HE21	1.63	0.63
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.80	0.63
1:L:107:LYS:HD2	9:L:8983:HOH:O	1.98	0.63
3:D:708:LEU:HD13	3:D:1231:GLU:HA	1.79	0.63
2:M:953:VAL:HG13	2:M:966:LEU:HD13	1.80	0.63
1:B:203:GLY:HA2	9:B:9589:HOH:O	1.99	0.63
2:C:731:GLU:HG3	9:C:9837:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1024:LYS:HB2	9:C:9932:HOH:O	1.97	0.63
3:N:440:VAL:HG23	9:N:9421:HOH:O	1.98	0.63
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.24	0.63
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.81	0.63
3:D:1394:VAL:HB	3:D:1397:LYS:HB2	1.80	0.63
2:C:1016:ILE:HD13	2:C:1016:ILE:H	1.63	0.63
3:N:441:ARG:HG2	9:N:9718:HOH:O	1.98	0.63
2:C:511:GLU:O	2:C:526:PRO:HD3	1.98	0.63
1:A:104:GLU:HG3	9:A:9611:HOH:O	1.99	0.63
1:A:18:ARG:O	1:A:207:PRO:HD3	1.99	0.63
3:N:107:ASP:HA	9:N:9514:HOH:O	1.99	0.63
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.79	0.63
1:K:178:ALA:HB3	1:K:198:ARG:HG3	1.80	0.63
2:M:528:GLU:HA	9:M:9431:HOH:O	1.99	0.63
3:N:1175:ILE:O	3:N:1179:GLU:HG3	1.97	0.63
2:M:164:PRO:HA	2:M:266:ARG:NH2	2.12	0.63
2:M:328:LEU:HA	9:M:9297:HOH:O	1.98	0.63
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.81	0.63
2:M:129:ILE:HG22	2:M:130:ASN:N	2.14	0.63
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.64	0.63
2:M:1057:SER:HB2	3:N:622:ARG:O	1.99	0.63
2:M:567:GLN:HB3	2:M:997:LEU:HD22	1.80	0.63
3:D:1215:VAL:HB	9:D:9841:HOH:O	1.99	0.63
3:N:65:ARG:CB	5:P:375:LEU:HA	2.26	0.63
5:P:402:ASN:HA	9:P:3207:HOH:O	1.99	0.63
3:D:86:ARG:O	3:D:522:PRO:HD2	1.99	0.63
2:M:129:ILE:HD11	9:M:9705:HOH:O	1.98	0.63
3:N:806:PHE:O	3:N:808:THR:N	2.32	0.63
1:L:212:ASN:HB2	9:L:1267:HOH:O	1.98	0.63
3:D:1150:ALA:O	3:D:1151:ARG:HD3	1.99	0.63
3:N:545:ARG:HD2	9:P:1680:HOH:O	1.98	0.63
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.81	0.63
3:N:598:ARG:HH11	3:N:598:ARG:HG2	1.63	0.63
3:D:574:LEU:O	3:D:578:VAL:HG23	1.99	0.63
4:O:94:PRO:HG2	9:O:6584:HOH:O	1.97	0.63
3:D:1209:LEU:HG	3:D:1211:MET:SD	2.39	0.62
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.33	0.62
3:D:1052:THR:HG23	9:D:2494:HOH:O	1.99	0.62
3:D:966:GLU:HA	3:D:969:ARG:NH1	2.14	0.62
1:K:14:ARG:HB3	9:K:1738:HOH:O	1.99	0.62
2:M:1104:GLU:HB2	9:M:2124:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:231:ARG:HB3	5:F:233:PHE:CE2	2.34	0.62
3:D:984:THR:HG22	3:D:987:GLU:CG	2.27	0.62
5:P:361:LEU:HB3	9:P:1329:HOH:O	1.98	0.62
3:N:1428:ALA:O	3:N:1431:THR:HG23	1.99	0.62
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.28	0.62
3:D:521:PRO:HB2	3:D:524:LEU:HD12	1.80	0.62
4:E:74:VAL:HG12	4:E:79:LEU:HD21	1.80	0.62
5:P:151:LEU:HB2	5:P:155:THR:OG1	1.99	0.62
1:K:39:PRO:O	1:K:43:ILE:HG12	1.99	0.62
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.80	0.62
3:D:988:ARG:HD2	9:D:9919:HOH:O	1.99	0.62
1:L:88:ARG:HB2	9:L:1335:HOH:O	1.97	0.62
3:D:1440:PHE:HB2	3:D:1442:ASN:ND2	2.15	0.62
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.33	0.62
3:N:1332:PRO:HD2	9:N:2721:HOH:O	1.98	0.62
1:K:100:LEU:HD12	1:K:115:LEU:HD21	1.81	0.62
3:D:1068:LEU:HG	3:D:1072:ILE:HG12	1.80	0.62
3:N:890:VAL:HG13	3:N:926:LYS:HD3	1.81	0.62
3:D:810:GLU:O	3:D:813:LEU:HG	2.00	0.62
3:N:103:TRP:HZ2	3:N:604:THR:HG23	1.63	0.62
2:M:1049:LEU:O	2:M:1053:LEU:HD23	1.99	0.62
1:B:176:ARG:HB2	9:B:9702:HOH:O	1.99	0.62
3:N:871:LYS:HE2	3:N:873:LEU:HD21	1.79	0.62
2:M:614:ARG:HG3	9:M:9292:HOH:O	2.00	0.62
3:D:1390:LEU:HA	9:D:9843:HOH:O	1.99	0.62
3:D:604:THR:HA	3:D:607:LEU:HD12	1.81	0.62
1:A:78:ILE:HA	9:A:9585:HOH:O	1.99	0.62
3:D:616:GLN:O	3:D:619:LEU:HB3	1.99	0.62
2:C:752:GLY:H	2:C:792:VAL:HB	1.64	0.62
3:N:1279:GLY:O	3:N:1318:TYR:HA	2.00	0.62
3:N:607:LEU:HD23	9:N:2546:HOH:O	1.99	0.62
3:D:563:PRO:HG3	5:F:188:ILE:HG21	1.80	0.62
3:D:1097:LYS:O	3:D:1101:VAL:HG23	1.99	0.62
3:D:972:LEU:HB2	9:D:2563:HOH:O	2.00	0.62
2:M:586:ARG:HB3	2:M:586:ARG:NH1	2.13	0.62
3:D:999:THR:HA	3:D:1002:LYS:HD2	1.82	0.62
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.81	0.62
3:N:146:PRO:HA	9:N:9595:HOH:O	1.99	0.62
3:D:551:ASN:HA	9:D:9809:HOH:O	1.99	0.62
3:N:684:LYS:HB3	3:N:686:GLU:OE2	2.00	0.62
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1262:LEU:HD23	3:D:1352:ILE:HG12	1.80	0.62
8:N:9101:G4P:H5"	8:N:9101:G4P:H8	1.80	0.62
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.99	0.62
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.64	0.62
3:N:1421:LEU:HA	9:N:9377:HOH:O	1.98	0.62
3:N:1034:GLN:HA	3:N:1037:GLN:NE2	2.14	0.62
2:C:516:ARG:CZ	3:D:1068:LEU:HD22	2.29	0.62
1:B:52:ALA:HB3	9:B:9602:HOH:O	1.98	0.62
1:L:108:GLU:HB2	9:L:1445:HOH:O	2.00	0.62
1:K:226:SER:O	1:K:228:PRO:HD3	1.98	0.62
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.63	0.62
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.82	0.62
2:M:719:PRO:HB3	9:M:9756:HOH:O	1.98	0.62
3:D:220:ARG:HA	9:D:9675:HOH:O	1.99	0.62
3:N:1394:VAL:HG13	9:N:2001:HOH:O	1.99	0.62
1:A:180:GLN:NE2	2:C:934:PHE:HB2	2.14	0.62
2:M:304:LEU:HB3	2:M:305:PRO:HD3	1.82	0.62
9:N:9288:HOH:O	4:O:54:LEU:HD11	2.00	0.62
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.00	0.62
3:N:1012:GLU:HG2	3:N:1021:TYR:OH	1.99	0.62
3:D:631:ILE:HG12	3:D:743:ASP:O	1.99	0.62
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.14	0.62
2:C:195:LEU:O	2:C:199:VAL:HG23	1.98	0.62
2:C:442:GLU:HG2	2:C:454:SER:CB	2.28	0.62
2:M:492:ASP:HB2	9:M:9314:HOH:O	1.99	0.62
3:N:1271:LYS:HG3	9:N:9632:HOH:O	2.00	0.62
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.00	0.62
2:M:758:ARG:HG3	9:M:9349:HOH:O	2.00	0.62
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.82	0.62
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.34	0.62
1:B:20:TYR:HB3	9:B:9603:HOH:O	1.99	0.62
1:B:206:THR:HG22	1:B:209:GLU:H	1.64	0.62
5:F:158:GLU:HA	5:F:161:GLN:CD	2.19	0.62
3:D:1378:TYR:OH	3:D:1431:THR:HG22	1.99	0.62
3:N:1046:GLN:OE1	3:N:1079:LYS:HD3	1.99	0.62
3:D:464:LEU:HA	9:D:9601:HOH:O	2.00	0.62
2:M:536:PRO:HB3	2:M:906:PHE:CD1	2.29	0.62
2:M:497:ALA:HA	2:M:515:ALA:HA	1.82	0.62
1:L:224:TYR:HB2	9:L:4548:HOH:O	1.98	0.62
2:C:773:LEU:O	2:C:777:ILE:HG13	2.00	0.62
5:P:166:LEU:HD13	5:P:170:HIS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG12	1:A:124:ASN:HD22	1.65	0.62
1:B:59:GLU:HG3	1:B:60:ASP:H	1.64	0.62
2:M:225:SER:HB2	9:M:2105:HOH:O	2.00	0.62
2:C:911:GLU:O	2:C:915:LYS:HG2	1.98	0.62
2:C:958:THR:HG22	9:C:2770:HOH:O	1.99	0.62
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.00	0.62
3:D:1243:THR:HB	3:D:1253:THR:HB	1.80	0.62
3:D:701:LEU:O	3:D:747:VAL:HG23	2.00	0.62
3:D:1046:GLN:HB3	3:D:1052:THR:HG22	1.81	0.62
2:C:186:VAL:HG23	2:C:187:ASN:H	1.64	0.62
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.82	0.62
3:D:502:PHE:CE2	3:D:1452:ILE:HG23	2.34	0.62
2:C:497:ALA:HA	2:C:515:ALA:HA	1.81	0.62
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.00	0.62
2:C:793:PRO:HB3	9:C:9926:HOH:O	1.99	0.62
2:M:911:GLU:HB3	2:M:912:PRO:HD3	1.82	0.61
3:D:148:GLU:HG3	9:D:3099:HOH:O	1.99	0.61
3:D:484:PRO:O	3:D:489:ARG:HD2	2.00	0.61
4:O:54:LEU:O	4:O:54:LEU:HD23	2.00	0.61
3:N:884:ARG:HD3	3:N:888:GLU:OE2	1.99	0.61
2:C:430:VAL:HG13	3:D:1075:HIS:HA	1.82	0.61
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.80	0.61
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.80	0.61
2:C:189:ARG:HB3	9:C:9840:HOH:O	1.99	0.61
3:D:152:LEU:HD23	3:D:152:LEU:H	1.64	0.61
2:M:610:ARG:HB2	9:M:9214:HOH:O	2.00	0.61
3:N:130:SER:HA	3:N:572:ARG:NH1	2.14	0.61
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.11	0.61
2:C:207:LEU:O	2:C:211:LEU:HB3	2.00	0.61
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.81	0.61
2:C:376:ARG:HB2	2:C:377:PRO:HD3	1.81	0.61
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	2.00	0.61
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.81	0.61
1:B:30:ARG:HD3	9:B:9697:HOH:O	2.00	0.61
2:M:220:GLY:HA3	9:M:9787:HOH:O	1.99	0.61
5:F:85:LEU:HD12	9:F:9829:HOH:O	2.00	0.61
1:A:197:LEU:HD23	1:A:197:LEU:H	1.66	0.61
1:B:117:VAL:HG21	9:B:9656:HOH:O	1.98	0.61
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.82	0.61
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.83	0.61
2:C:28:ARG:HG3	9:C:2013:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:394:ARG:HD3	9:F:2104:HOH:O	1.99	0.61
2:C:327:HIS:HB3	2:C:330:ASN:HD22	1.65	0.61
1:L:73:GLU:HB3	9:L:1341:HOH:O	1.98	0.61
3:D:39:PRO:HB3	3:D:45:PHE:O	2.00	0.61
2:C:909:ALA:HB1	2:C:914:ILE:HD11	1.83	0.61
2:M:961:GLU:HG2	9:M:2341:HOH:O	2.00	0.61
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.81	0.61
4:O:40:LEU:HB3	9:O:2072:HOH:O	2.00	0.61
2:M:1054:THR:HG23	2:M:1059:ASP:HB2	1.81	0.61
1:A:42:ARG:HD3	1:B:35:THR:HG23	1.83	0.61
3:N:87:ARG:HD3	3:N:523:ASP:OD2	2.00	0.61
3:N:434:ARG:HG3	9:N:9455:HOH:O	2.00	0.61
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.81	0.61
3:D:1438:ALA:O	3:D:1443:THR:HG22	2.00	0.61
1:K:18:ARG:O	1:K:207:PRO:HD3	2.00	0.61
3:D:664:LYS:HG2	9:D:2544:HOH:O	2.00	0.61
3:D:1310:ARG:HD2	9:D:2631:HOH:O	2.00	0.61
3:N:568:ARG:HA	3:N:571:LYS:HE3	1.82	0.61
2:M:141:HIS:O	2:M:331:ARG:HA	2.00	0.61
3:D:191:LEU:HD13	3:D:195:VAL:HG11	1.83	0.61
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.35	0.61
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.00	0.61
5:F:271:LEU:HD23	5:F:295:MET:HG3	1.82	0.61
3:D:1197:ARG:HH12	3:D:1377:LYS:HB2	1.66	0.61
2:M:1013:TYR:CE2	5:P:341:PRO:HD2	2.34	0.61
2:M:412:ALA:HB1	2:M:419:THR:HG21	1.81	0.61
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.35	0.61
1:A:36:LEU:O	1:A:39:PRO:HD2	2.01	0.61
3:N:1403:LEU:HA	9:N:9392:HOH:O	2.00	0.61
1:L:20:TYR:OH	1:L:198:ARG:HD2	1.99	0.61
5:P:308:LEU:O	5:P:312:GLN:HG3	2.01	0.61
3:N:81:THR:HB	3:N:85:VAL:CG2	2.31	0.61
2:C:794:PRO:HB3	9:C:2362:HOH:O	1.99	0.61
5:P:353:GLU:HG2	5:P:417:LYS:HB3	1.81	0.61
5:P:148:LYS:HA	9:P:1661:HOH:O	2.00	0.61
1:L:66:SER:HA	9:L:6317:HOH:O	1.99	0.61
3:D:895:VAL:O	3:D:899:LEU:HD12	2.01	0.61
3:N:2:LYS:HB2	9:N:9489:HOH:O	2.00	0.61
3:D:3:LYS:H	3:D:3:LYS:HD3	1.65	0.61
1:B:128:HIS:HB3	9:B:9670:HOH:O	2.00	0.61
2:M:496:ILE:HG12	2:M:531:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:991:GLN:HA	9:N:9221:HOH:O	2.00	0.61
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.81	0.61
3:N:1389:LEU:H	3:N:1389:LEU:CD2	2.12	0.61
5:F:308:LEU:O	5:F:312:GLN:HG2	2.01	0.61
2:M:195:LEU:HB3	2:M:238:LEU:HD21	1.81	0.61
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.82	0.61
3:D:580:ALA:HA	3:D:584:ASN:OD1	2.00	0.61
5:P:94:LEU:HD12	5:P:97:GLU:N	2.15	0.61
2:C:1069:ALA:O	2:C:1074:GLU:HG2	2.01	0.61
2:C:413:LEU:HD12	2:C:413:LEU:H	1.66	0.61
1:A:96:THR:HG21	9:A:9575:HOH:O	2.00	0.61
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.30	0.61
2:M:87:ASP:HB3	9:M:9773:HOH:O	2.00	0.61
5:F:192:LEU:O	5:F:196:VAL:HG23	2.01	0.61
2:C:958:THR:HG23	2:C:961:GLU:HB2	1.82	0.61
1:K:17:GLY:HA3	9:K:3120:HOH:O	2.00	0.61
1:A:227:ASN:H	1:A:227:ASN:HD22	1.48	0.61
1:A:223:THR:HB	9:A:9644:HOH:O	2.00	0.61
3:N:1342:GLU:HB2	9:N:2770:HOH:O	1.99	0.61
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.83	0.61
2:M:189:ARG:HH21	2:M:243:ARG:NH2	1.98	0.61
2:M:910:LYS:HB3	9:M:9220:HOH:O	2.01	0.61
1:A:30:ARG:HH22	1:B:155:LYS:NZ	1.98	0.61
2:C:1049:LEU:O	2:C:1053:LEU:HD23	2.00	0.61
2:C:21:ILE:HD12	2:C:21:ILE:H	1.66	0.61
2:C:762:LYS:HE2	2:C:771:GLU:OE1	2.01	0.61
3:D:1115:THR:HB	9:D:2390:HOH:O	2.01	0.61
5:P:122:LEU:HG	5:P:126:LEU:HD23	1.83	0.61
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.82	0.61
3:D:172:PRO:HD2	3:D:389:GLU:O	2.00	0.61
5:P:393:THR:HG22	5:P:394:ARG:N	2.16	0.61
3:N:836:VAL:HG13	9:N:9636:HOH:O	2.01	0.61
2:M:647:GLN:HA	9:M:9256:HOH:O	2.00	0.61
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.31	0.61
5:F:370:LYS:HE3	5:F:371:LEU:HG	1.83	0.61
5:P:372:ARG:HB3	9:P:2070:HOH:O	2.00	0.61
3:D:14:SER:HB2	3:D:17:LYS:HG3	1.83	0.61
1:B:7:LYS:HB3	1:B:7:LYS:NZ	2.16	0.61
5:P:297:PRO:HA	9:P:7238:HOH:O	2.01	0.61
3:D:86:ARG:NH1	3:D:522:PRO:HB2	2.16	0.60
2:C:724:ARG:HG3	9:C:9568:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:743:ASP:HA	9:N:9297:HOH:O	2.00	0.60
2:M:721:ARG:HH21	2:M:783:ARG:HH21	1.48	0.60
2:C:507:ARG:HH11	2:C:507:ARG:HB2	1.65	0.60
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.83	0.60
2:M:96:ALA:HB2	9:M:9250:HOH:O	2.00	0.60
2:C:1034:GLU:HG2	9:C:9872:HOH:O	2.01	0.60
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.82	0.60
2:M:730:SER:O	2:M:734:LEU:HD23	2.01	0.60
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.01	0.60
5:F:191:ASN:HA	9:F:9560:HOH:O	2.00	0.60
3:D:1044:LEU:HA	9:D:2083:HOH:O	2.00	0.60
2:M:881:ASN:H	2:M:881:ASN:HD22	1.47	0.60
2:C:328:LEU:HD11	2:C:434:HIS:CD2	2.36	0.60
2:M:71:TYR:HB2	9:M:9393:HOH:O	2.01	0.60
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.82	0.60
2:C:1115:LEU:HD22	3:D:88:TYR:HD1	1.65	0.60
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.16	0.60
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.66	0.60
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.36	0.60
2:C:893:ALA:HB1	9:C:9860:HOH:O	1.99	0.60
2:M:1004:LYS:HE3	2:M:1027:PHE:HE1	1.66	0.60
2:C:18:LEU:HD12	2:C:18:LEU:H	1.67	0.60
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.66	0.60
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.83	0.60
2:C:1087:VAL:HG12	2:C:1091:GLU:OE1	2.01	0.60
3:N:98:PRO:HG2	3:N:462:GLN:NE2	2.15	0.60
5:P:142:ARG:NH1	5:P:142:ARG:HB3	2.16	0.60
2:C:838:LYS:HB3	2:C:848:VAL:HG22	1.82	0.60
3:N:838:ARG:HB3	9:N:9286:HOH:O	2.00	0.60
3:N:1258:ARG:CZ	3:N:1262:LEU:HD11	2.30	0.60
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.67	0.60
3:D:864:VAL:HG12	3:D:865:THR:H	1.66	0.60
2:M:707:ARG:HG2	9:M:9461:HOH:O	2.02	0.60
1:A:227:ASN:HD22	1:A:227:ASN:N	2.00	0.60
3:D:17:LYS:HG2	9:D:2736:HOH:O	2.02	0.60
2:C:432:ARG:HG3	2:C:432:ARG:HH11	1.66	0.60
5:P:225:GLU:HB3	5:P:226:LYS:HZ2	1.65	0.60
3:D:119:SER:HB2	3:D:123:LEU:N	2.13	0.60
3:N:177:ALA:HA	3:N:199:LEU:HD13	1.83	0.60
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	2.01	0.60
1:L:123:MET:HG3	9:L:2931:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.82	0.60
1:K:44:LEU:HD23	1:K:48:ILE:HD11	1.83	0.60
1:A:227:ASN:ND2	1:A:227:ASN:H	2.00	0.60
3:D:1406:ARG:HA	9:D:9597:HOH:O	2.01	0.60
2:C:15:LEU:HD22	9:C:9604:HOH:O	2.01	0.60
5:P:198:ILE:HA	9:P:8888:HOH:O	2.01	0.60
1:L:226:SER:O	1:L:228:PRO:HD3	2.02	0.60
3:N:490:ALA:HA	9:N:9668:HOH:O	1.99	0.60
1:B:67:THR:HA	9:B:9649:HOH:O	2.02	0.60
1:L:162:ILE:HG12	9:L:4752:HOH:O	2.00	0.60
3:D:754:PHE:HE2	3:D:1476:THR:HG21	1.66	0.60
3:D:493:ARG:CD	3:D:1390:LEU:HD21	2.31	0.60
2:M:1096:ALA:O	3:N:13:ALA:HB2	2.01	0.60
3:D:500:ARG:HH22	3:D:1388:ARG:HE	1.50	0.60
3:N:123:LEU:HD11	3:N:152:LEU:HD22	1.84	0.60
3:D:536:ALA:HA	5:F:315:VAL:O	2.01	0.60
2:M:203:ASP:O	2:M:207:LEU:HB2	2.01	0.60
2:C:833:LEU:HD11	2:C:849:VAL:HG21	1.84	0.60
3:N:858:VAL:HA	9:N:9450:HOH:O	1.99	0.60
3:N:1258:ARG:HG2	3:N:1262:LEU:HD13	1.82	0.60
1:K:211:LEU:O	1:K:215:VAL:HG13	2.01	0.60
1:A:134:GLU:HB3	9:A:9569:HOH:O	2.01	0.60
2:M:69:LEU:HD12	2:M:97:ARG:HB3	1.83	0.60
3:D:719:VAL:O	3:D:721:VAL:HG13	2.01	0.60
2:M:234:ALA:HB1	9:M:9363:HOH:O	2.01	0.60
1:B:73:GLU:HA	9:B:9614:HOH:O	2.01	0.60
3:N:9:ARG:NH1	3:N:11:ALA:HB2	2.15	0.60
2:C:208:ALA:HB3	9:C:9874:HOH:O	2.01	0.60
3:N:486:ARG:HH21	3:N:489:ARG:NE	2.00	0.60
1:K:110:LYS:HD3	9:K:1727:HOH:O	2.01	0.60
2:M:221:LEU:HG	9:M:9323:HOH:O	2.02	0.60
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.16	0.60
3:N:728:LEU:HD22	3:N:745:MET:SD	2.42	0.60
3:N:817:GLU:O	3:N:821:VAL:HG23	2.01	0.60
3:N:1301:LYS:HD2	9:N:9307:HOH:O	2.00	0.60
5:F:234:LYS:HB2	9:F:9575:HOH:O	2.01	0.60
3:N:1290:LEU:HD22	9:N:9440:HOH:O	2.00	0.60
1:A:23:PHE:HE1	1:A:208:LEU:HD22	1.67	0.60
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.01	0.60
3:N:902:LEU:HD11	9:N:2304:HOH:O	2.00	0.60
2:C:204:GLN:HB3	2:C:222:MET:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:598:ARG:HB2	9:D:3283:HOH:O	2.00	0.60
5:P:363:GLU:O	5:P:367:MET:HG2	2.02	0.60
2:C:218:VAL:HG11	9:C:9905:HOH:O	2.01	0.60
3:D:625:TYR:O	3:D:749:VAL:HG23	2.01	0.60
2:C:1106:ASP:HA	9:C:9776:HOH:O	2.00	0.60
5:F:369:LEU:HD23	9:F:2056:HOH:O	2.01	0.60
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.17	0.60
2:C:722:ILE:HG21	2:C:821:GLU:OE1	2.02	0.60
5:P:93:LEU:HG	5:P:190:ALA:CB	2.32	0.60
3:D:1314:LYS:HA	9:D:2549:HOH:O	2.00	0.60
2:C:1002:GLU:HG3	3:D:744:GLN:HE22	1.66	0.60
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.83	0.60
2:C:881:ASN:HD22	2:C:881:ASN:H	1.47	0.60
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.82	0.60
5:F:138:SER:O	5:F:141:VAL:HG12	2.01	0.60
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.01	0.60
3:D:462:GLN:HG2	3:D:466:LYS:HE3	1.82	0.60
2:M:370:ALA:HB1	5:P:280:GLN:HB2	1.83	0.60
2:M:295:ASP:HB2	9:M:2030:HOH:O	2.01	0.60
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.82	0.60
5:P:367:MET:HB3	5:P:370:LYS:NZ	2.17	0.60
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.41	0.60
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.83	0.60
3:N:654:LYS:HD3	3:N:674:ARG:NH1	2.16	0.60
3:N:698:LYS:HG3	4:O:59:ASN:HD21	1.67	0.60
3:D:616:GLN:HB2	5:F:326:ASP:HB2	1.84	0.60
3:D:1415:VAL:HG21	9:D:9816:HOH:O	2.01	0.60
1:L:73:GLU:HG3	1:L:130:ALA:HA	1.84	0.60
2:M:660:ALA:HB1	2:M:667:ALA:O	2.02	0.60
5:F:102:LEU:HB2	5:F:187:LEU:HD12	1.84	0.60
3:D:240:GLU:HA	9:D:3064:HOH:O	2.00	0.60
2:M:480:THR:HG22	2:M:482:GLU:H	1.66	0.60
2:M:946:ARG:HD2	2:M:984:GLU:HB2	1.83	0.60
5:F:92:PRO:HB2	9:F:9606:HOH:O	2.02	0.60
4:O:40:LEU:HB2	4:O:45:ARG:NE	2.17	0.59
5:P:361:LEU:HD11	5:P:408:LEU:HD13	1.84	0.59
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	1.84	0.59
3:N:98:PRO:O	3:N:458:ALA:HB3	2.02	0.59
2:C:1013:TYR:HB3	2:C:1018:GLN:HE21	1.66	0.59
4:E:47:LYS:HD3	9:E:9670:HOH:O	2.02	0.59
3:D:565:ILE:HG21	5:F:84:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1100:ASP:HB3	3:D:1440:PHE:HZ	1.66	0.59
1:B:191:ASP:HB2	9:B:9697:HOH:O	2.02	0.59
1:A:100:LEU:HD12	1:A:115:LEU:HD21	1.83	0.59
3:D:131:LYS:HA	3:D:456:MET:HG3	1.84	0.59
3:D:1380:GLU:HG2	9:D:9843:HOH:O	2.02	0.59
2:M:266:ARG:CD	2:M:288:ARG:HH12	2.14	0.59
2:C:405:ARG:HH22	2:C:409:ARG:NH2	1.99	0.59
3:D:195:VAL:HB	3:D:205:TYR:HB2	1.84	0.59
3:D:119:SER:H	3:D:123:LEU:CD1	2.15	0.59
3:N:116:LEU:HD11	3:N:465:LEU:HG	1.84	0.59
3:D:592:THR:HG21	9:D:9883:HOH:O	2.00	0.59
2:M:874:LEU:HD13	3:N:783:ARG:HB3	1.84	0.59
1:A:219:ARG:NH1	1:B:219:ARG:HG2	2.18	0.59
2:C:69:LEU:HB3	9:C:9789:HOH:O	2.01	0.59
2:M:172:ILE:HG12	2:M:186:VAL:HG12	1.84	0.59
2:C:453:THR:HA	9:C:9566:HOH:O	2.02	0.59
3:N:1149:LEU:HD11	3:N:1160:LEU:HB3	1.84	0.59
2:M:499:ALA:HA	2:M:532:MET:HE3	1.85	0.59
3:D:488:ARG:HB3	3:D:488:ARG:NH1	2.18	0.59
5:P:323:ASP:O	5:P:325:LYS:HG2	2.02	0.59
3:N:574:LEU:O	3:N:578:VAL:HG23	2.02	0.59
2:C:585:GLU:HB3	2:C:589:ARG:HH22	1.66	0.59
5:F:415:THR:O	5:F:417:LYS:HG3	2.01	0.59
3:N:9:ARG:HD3	3:N:1456:LYS:CG	2.32	0.59
3:N:9:ARG:HG3	3:N:1455:LYS:O	2.03	0.59
3:N:1189:ARG:HB3	3:N:1189:ARG:NH1	2.16	0.59
1:K:72:LYS:HZ1	2:M:644:VAL:HA	1.68	0.59
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.32	0.59
2:M:579:VAL:CG1	2:M:887:GLU:HG3	2.32	0.59
3:N:473:LEU:HD13	9:N:9510:HOH:O	2.02	0.59
2:M:19:THR:HG21	2:M:124:ASP:O	2.02	0.59
3:D:1097:LYS:HB3	9:D:9630:HOH:O	2.03	0.59
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.84	0.59
2:M:1054:THR:HG22	2:M:1055:LEU:N	2.17	0.59
2:M:1055:LEU:HD22	2:M:1066:ALA:HB2	1.84	0.59
2:M:507:ARG:HG3	9:M:9830:HOH:O	2.02	0.59
4:E:23:VAL:HG21	9:E:9593:HOH:O	2.03	0.59
2:C:266:ARG:HB3	9:C:9842:HOH:O	2.01	0.59
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.01	0.59
2:C:787:ASP:HA	9:C:9784:HOH:O	2.01	0.59
3:D:487:ALA:HB3	3:D:488:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:HB3	9:C:2301:HOH:O	2.02	0.59
2:C:814:GLU:HA	9:C:9961:HOH:O	2.01	0.59
3:N:598:ARG:HG2	3:N:598:ARG:NH1	2.17	0.59
2:C:921:ALA:HA	9:C:2761:HOH:O	2.02	0.59
2:C:728:HIS:HB3	2:C:729:LEU:HD22	1.84	0.59
1:A:226:SER:O	1:A:228:PRO:HD3	2.01	0.59
3:N:84:ILE:HG22	9:N:9289:HOH:O	2.03	0.59
3:D:496:LEU:HG	3:D:500:ARG:HG2	1.85	0.59
3:N:131:LYS:HB3	3:N:568:ARG:HG2	1.83	0.59
3:D:781:PRO:HG2	3:D:911:LEU:HD23	1.83	0.59
3:D:171:LEU:HD13	3:D:389:GLU:C	2.23	0.59
2:C:165:LEU:HD22	2:C:418:LEU:HD11	1.84	0.59
1:K:2:LEU:HA	1:K:6:LEU:HD22	1.84	0.59
1:L:59:GLU:HG3	1:L:60:ASP:H	1.67	0.59
3:N:1379:VAL:HG11	3:N:1395:LEU:HD23	1.84	0.59
1:A:92:PRO:HA	9:A:9625:HOH:O	2.02	0.59
2:C:145:GLY:H	2:C:163:ILE:HG23	1.67	0.59
3:D:132:TYR:HA	9:D:9996:HOH:O	2.01	0.59
2:M:369:PRO:HA	9:M:9861:HOH:O	2.03	0.59
2:C:660:ALA:HB1	2:C:667:ALA:O	2.03	0.59
2:M:569:VAL:HG12	2:M:996:LYS:O	2.03	0.59
3:N:662:GLU:OE2	3:N:669:ASN:HA	2.03	0.59
5:P:181:GLU:O	5:P:184:ARG:HB3	2.01	0.59
5:P:316:SER:OG	5:P:318:GLU:HG3	2.02	0.59
1:K:212:ASN:O	1:K:215:VAL:HG22	2.03	0.59
2:M:63:GLY:HA3	2:M:103:LYS:HG2	1.85	0.59
3:N:1114:THR:CG2	3:N:1195:GLN:HB2	2.32	0.59
3:N:1014:ASN:HB3	9:N:9749:HOH:O	2.02	0.59
3:D:800:LYS:HE2	3:D:830:ALA:HB3	1.84	0.59
1:K:192:LEU:HG	9:K:2051:HOH:O	2.01	0.59
3:D:1489:GLN:HB2	9:D:9922:HOH:O	2.02	0.59
2:C:35:PRO:HD2	2:C:38:LYS:HE2	1.83	0.59
2:M:691:SER:HB2	2:M:858:MET:SD	2.43	0.59
2:C:710:ILE:CD1	2:C:758:ARG:HE	2.12	0.59
2:M:230:ARG:HE	2:M:237:ARG:HH22	1.48	0.59
2:M:769:PRO:HA	9:M:9896:HOH:O	2.02	0.59
3:N:39:PRO:HB3	3:N:45:PHE:C	2.23	0.59
2:C:184:MET:CE	2:C:186:VAL:HG13	2.32	0.59
9:C:2004:HOH:O	4:E:31:LEU:HD23	2.03	0.59
3:N:1114:THR:HB	3:N:1195:GLN:OE1	2.02	0.59
2:M:927:GLY:HA2	2:M:930:LYS:NZ	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:386:PHE:HA	9:M:9269:HOH:O	2.01	0.59
3:N:550:ARG:HG3	3:N:550:ARG:HH11	1.68	0.59
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.82	0.59
2:C:761:PHE:HB3	9:C:9910:HOH:O	2.01	0.59
1:B:102:LYS:HD3	9:B:9822:HOH:O	2.03	0.59
5:F:282:LEU:HD12	5:F:284:ARG:HB2	1.84	0.59
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.32	0.59
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.84	0.59
3:D:770:LEU:HD11	3:D:919:PHE:CE2	2.38	0.59
2:M:12:VAL:HG13	2:M:13:ILE:HG12	1.85	0.59
2:C:386:PHE:HA	9:C:9782:HOH:O	2.02	0.59
2:M:1001:VAL:HG23	9:M:9493:HOH:O	2.02	0.59
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.03	0.59
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.67	0.59
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.85	0.59
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.67	0.59
5:P:113:ILE:HG23	5:P:127:ILE:HB	1.84	0.59
2:C:328:LEU:HD22	2:C:433:THR:O	2.03	0.59
3:D:1459:LEU:HB3	3:D:1465:ASN:HD22	1.67	0.59
2:M:144:PRO:O	2:M:276:LYS:HD3	2.03	0.59
2:M:837:ASP:HA	9:M:9267:HOH:O	2.03	0.59
3:N:1374:GLN:OE1	3:N:1377:LYS:HD3	2.02	0.59
3:N:703:ASN:ND2	3:N:713:ILE:HG12	2.18	0.59
1:B:212:ASN:O	1:B:215:VAL:HG22	2.03	0.59
3:N:605:ASP:HA	3:N:610:LYS:HG3	1.85	0.59
3:D:1440:PHE:HB2	3:D:1442:ASN:HD21	1.66	0.59
3:N:19:ARG:HG3	9:N:9537:HOH:O	2.02	0.59
3:D:565:ILE:HD12	3:D:565:ILE:H	1.68	0.58
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.85	0.58
3:N:499:VAL:O	3:N:503:LEU:HB2	2.03	0.58
5:F:132:ARG:HH21	5:F:184:ARG:HH12	1.51	0.58
3:N:1096:ARG:NH1	3:N:1096:ARG:HB2	2.17	0.58
3:N:887:ALA:HA	9:N:9628:HOH:O	2.03	0.58
3:N:119:SER:HB2	3:N:123:LEU:N	2.17	0.58
4:O:54:LEU:HD12	9:O:3002:HOH:O	2.02	0.58
2:M:537:LYS:HA	2:M:545:ASN:ND2	2.17	0.58
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.85	0.58
3:N:957:PRO:HB3	3:N:1010:ASN:HD22	1.68	0.58
5:P:93:LEU:HD22	5:P:98:GLU:HB3	1.85	0.58
2:C:44:ILE:HG13	2:C:344:PHE:CE2	2.38	0.58
2:M:374:ASN:O	2:M:377:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1364:HIS:CE1	3:N:1366:LYS:HG3	2.37	0.58
3:D:430:ASP:HB2	9:D:2014:HOH:O	2.03	0.58
9:C:9643:HOH:O	3:D:532:GLY:HA2	2.03	0.58
2:M:420:ARG:HD2	2:M:420:ARG:H	1.68	0.58
2:C:964:LYS:HE3	9:C:2189:HOH:O	2.02	0.58
3:N:197:SER:CB	3:N:203:ALA:HB3	2.33	0.58
3:D:489:ARG:NE	3:D:493:ARG:HH22	1.95	0.58
5:P:371:LEU:HB2	9:P:5682:HOH:O	2.02	0.58
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.84	0.58
2:M:258:TYR:HB3	9:M:2121:HOH:O	2.02	0.58
1:A:178:ALA:HB2	2:C:864:GLY:H	1.66	0.58
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.38	0.58
2:C:1074:GLU:HA	9:C:2004:HOH:O	2.02	0.58
3:N:896:ALA:HB2	9:N:9628:HOH:O	2.03	0.58
3:D:1152:GLU:HG2	3:D:1159:ARG:HH21	1.67	0.58
2:C:225:SER:O	2:C:229:MET:HG2	2.04	0.58
2:M:909:ALA:HB1	2:M:914:ILE:HD11	1.85	0.58
3:D:1209:LEU:HD12	3:D:1210:SER:N	2.10	0.58
3:D:702:LEU:HD13	3:D:716:PHE:CD1	2.38	0.58
3:D:1390:LEU:H	3:D:1390:LEU:HD23	1.68	0.58
2:C:412:ALA:HB1	2:C:419:THR:HG21	1.86	0.58
5:P:339:PRO:HB3	5:P:343:ASP:HB2	1.84	0.58
3:N:432:TYR:HA	3:N:448:GLU:O	2.03	0.58
4:O:48:MET:HG2	4:O:49:GLN:H	1.67	0.58
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.85	0.58
3:N:794:GLN:HG2	3:N:905:PRO:HB3	1.85	0.58
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.03	0.58
1:K:89:PHE:HB3	1:K:94:LEU:HD13	1.85	0.58
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.68	0.58
3:N:820:GLU:HA	3:N:825:ALA:O	2.03	0.58
2:M:3:ILE:HA	2:M:900:ARG:O	2.04	0.58
3:D:1131:SER:HB2	9:D:2660:HOH:O	2.02	0.58
3:N:464:LEU:O	3:N:468:LEU:HG	2.03	0.58
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.85	0.58
9:K:2958:HOH:O	2:M:830:LYS:HD2	2.03	0.58
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.86	0.58
1:K:229:GLN:HG2	9:K:3118:HOH:O	2.02	0.58
2:M:954:THR:HG22	9:M:2147:HOH:O	2.03	0.58
2:C:1103:ASP:CG	2:C:1104:GLU:H	2.06	0.58
3:D:1282:ARG:NH1	3:D:1282:ARG:HB3	2.17	0.58
5:P:209:PHE:HA	5:P:212:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:GLU:HB3	9:D:9684:HOH:O	2.03	0.58
3:D:1433:SER:HB2	3:D:1457:ASP:OD2	2.04	0.58
3:D:1389:LEU:HG	3:D:1390:LEU:H	1.69	0.58
3:N:65:ARG:CG	3:N:66:GLN:H	2.16	0.58
5:P:371:LEU:HB3	9:P:1119:HOH:O	2.02	0.58
3:N:481:MET:O	3:N:489:ARG:HB2	2.03	0.58
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.02	0.58
3:N:441:ARG:HB3	3:N:443:VAL:CG2	2.33	0.58
2:C:810:ASP:HB3	2:C:813:VAL:HG22	1.84	0.58
3:D:799:LYS:HG2	3:D:826:PRO:CG	2.34	0.58
3:D:378:ILE:HA	9:D:2848:HOH:O	2.02	0.58
1:L:12:THR:OG1	1:L:24:VAL:HB	2.03	0.58
2:C:95:TYR:HD2	2:C:114:PHE:HB3	1.67	0.58
3:D:481:MET:O	3:D:489:ARG:HB2	2.02	0.58
2:C:627:ARG:HD2	9:C:9630:HOH:O	2.02	0.58
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.86	0.58
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.38	0.58
2:C:402:SER:HA	2:C:566:THR:HG23	1.86	0.58
3:D:761:ILE:HD12	4:E:20:THR:HG23	1.84	0.58
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.85	0.58
3:D:32:ILE:HA	9:D:2671:HOH:O	2.04	0.58
2:M:24:GLU:HB3	9:M:9330:HOH:O	2.03	0.58
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.85	0.58
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.03	0.58
4:O:50:THR:HA	9:O:2107:HOH:O	2.03	0.58
1:A:89:PHE:HB3	1:A:94:LEU:HD13	1.85	0.58
1:K:191:ASP:HA	9:K:2079:HOH:O	2.03	0.58
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.86	0.58
3:D:205:TYR:HE2	3:D:211:VAL:HG11	1.69	0.58
2:M:148:PHE:CB	2:M:313:LEU:HD22	2.32	0.58
2:M:1093:GLN:HE22	2:M:1098:ASP:HA	1.69	0.58
1:K:110:LYS:HB2	9:K:1330:HOH:O	2.04	0.58
1:K:217:ILE:HA	9:K:3364:HOH:O	2.02	0.58
3:N:1116:ASN:CG	3:N:1193:THR:HB	2.23	0.58
4:O:8:LYS:O	4:O:12:MET:HG3	2.04	0.58
5:F:369:LEU:HA	9:F:2056:HOH:O	2.03	0.58
3:N:539:ASP:HB2	5:P:318:GLU:OE2	2.03	0.58
3:N:580:ALA:HA	3:N:584:ASN:OD1	2.03	0.58
3:N:774:SER:HB3	3:N:1362:LYS:O	2.03	0.58
1:A:113:ASP:HB3	9:A:9594:HOH:O	2.02	0.58
3:D:1264:GLU:HG3	9:D:9596:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1049:SER:HA	9:N:9571:HOH:O	2.01	0.58
2:M:250:ARG:HE	2:M:253:ALA:HB3	1.66	0.58
2:C:129:ILE:HG22	2:C:130:ASN:N	2.18	0.58
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.85	0.58
4:E:63:TRP:O	4:E:67:GLU:HG3	2.04	0.58
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.86	0.58
2:M:897:LEU:HD11	2:M:920:GLN:HG3	1.86	0.58
3:N:1493:LYS:HB2	9:N:2722:HOH:O	2.03	0.58
3:N:710:ARG:HD2	9:N:9333:HOH:O	2.03	0.58
2:M:853:LEU:HB3	2:M:858:MET:HE3	1.85	0.58
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.69	0.58
4:O:58:PRO:HB2	9:O:4249:HOH:O	2.04	0.58
5:P:156:VAL:HG21	9:P:2305:HOH:O	2.03	0.58
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.33	0.58
4:E:40:LEU:HB2	4:E:45:ARG:NE	2.19	0.58
2:C:526:PRO:HB2	9:C:2408:HOH:O	2.03	0.58
2:C:250:ARG:HH21	2:C:254:VAL:H	1.52	0.58
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.38	0.58
3:D:456:MET:HG2	3:D:568:ARG:HH11	1.69	0.58
5:P:234:LYS:HG2	9:P:1255:HOH:O	2.02	0.58
1:A:229:GLN:HB2	9:A:9707:HOH:O	2.02	0.58
3:N:92:HIS:HA	3:N:519:VAL:HG23	1.85	0.58
5:F:265:VAL:HB	9:F:9892:HOH:O	2.04	0.58
3:N:149:LYS:HB2	9:N:9232:HOH:O	2.03	0.58
3:N:891:GLU:HB3	9:N:9355:HOH:O	2.04	0.58
3:N:692:GLU:OE1	3:N:720:LEU:HB2	2.04	0.58
4:E:44:GLU:O	4:E:45:ARG:HD3	2.04	0.58
4:E:60:ALA:O	4:E:63:TRP:HB2	2.04	0.58
3:N:559:ALA:HA	9:N:9528:HOH:O	2.03	0.58
3:D:28:LYS:HD2	3:D:41:ARG:HH11	1.68	0.58
1:A:18:ARG:HH22	1:A:88:ARG:HH21	1.51	0.58
3:N:137:PRO:HD2	3:N:453:ASP:HB3	1.86	0.58
2:M:244:PRO:HD2	2:M:245:GLY:H	1.68	0.58
2:C:807:ARG:HD3	2:C:808:ARG:O	2.03	0.58
5:F:208:SER:HA	9:F:9649:HOH:O	2.03	0.58
2:M:554:ASP:HB2	2:M:880:MET:HB2	1.85	0.58
2:C:943:VAL:HG13	2:C:985:GLY:H	1.68	0.58
3:N:707:THR:HA	9:N:2395:HOH:O	2.04	0.58
9:D:2101:HOH:O	4:E:48:MET:HA	2.04	0.57
9:N:9746:HOH:O	5:P:141:VAL:HG21	2.03	0.57
3:D:434:ARG:HB3	9:D:9861:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:LEU:HD11	1:L:138:LEU:HD13	1.85	0.57
2:M:481:ASP:HA	9:M:9383:HOH:O	2.04	0.57
2:M:371:LYS:O	2:M:372:LEU:HD12	2.04	0.57
2:M:564:MET:SD	2:M:846:LYS:HE2	2.44	0.57
2:M:791:ARG:HB3	9:M:9305:HOH:O	2.03	0.57
3:D:1240:THR:HG22	9:D:2840:HOH:O	2.03	0.57
3:N:1487:VAL:HG12	3:N:1488:ASP:N	2.19	0.57
3:N:1404:ASN:HB3	9:N:9535:HOH:O	2.04	0.57
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.86	0.57
3:D:489:ARG:HG3	3:D:493:ARG:NH1	2.11	0.57
2:M:142:ARG:HA	9:M:9253:HOH:O	2.04	0.57
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.86	0.57
3:N:430:ASP:HB2	3:N:432:TYR:CZ	2.39	0.57
2:C:1021:LEU:HG	2:C:1022:GLY:N	2.18	0.57
3:D:131:LYS:HE2	3:D:568:ARG:HG2	1.86	0.57
5:F:148:LYS:HA	9:F:9564:HOH:O	2.03	0.57
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.39	0.57
3:N:1209:LEU:HD21	4:O:16:LYS:HD2	1.85	0.57
2:M:107:LEU:HD12	9:M:9281:HOH:O	2.03	0.57
3:N:1025:GLN:HB2	9:N:2440:HOH:O	2.04	0.57
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.03	0.57
2:C:213:ALA:HB3	9:C:2338:HOH:O	2.04	0.57
5:P:406:ARG:HG3	9:P:3208:HOH:O	2.03	0.57
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.36	0.57
3:N:426:LYS:HB3	5:P:134:LYS:O	2.03	0.57
2:M:1093:GLN:HE22	2:M:1099:VAL:H	1.52	0.57
1:B:18:ARG:O	1:B:207:PRO:HD3	2.04	0.57
4:E:51:LEU:HD12	4:E:52:GLU:N	2.19	0.57
3:D:28:LYS:HB2	9:D:9655:HOH:O	2.04	0.57
3:N:539:ASP:HB2	5:P:318:GLU:CD	2.24	0.57
3:N:875:THR:HG22	3:N:879:ARG:HG3	1.86	0.57
2:C:4:LYS:HD2	9:C:2407:HOH:O	2.05	0.57
3:N:1412:LYS:O	3:N:1414:PRO:HD3	2.03	0.57
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.87	0.57
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.33	0.57
2:C:332:ARG:HD2	2:C:464:LEU:HG	1.86	0.57
1:K:92:PRO:HD3	9:K:1224:HOH:O	2.05	0.57
5:F:416:ARG:HD2	5:F:419:ARG:CB	2.34	0.57
3:N:394:LEU:HA	9:N:9499:HOH:O	2.03	0.57
1:L:152:PRO:HD2	1:L:155:LYS:CD	2.33	0.57
3:N:1195:GLN:HA	9:N:2116:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:551:ASN:O	3:N:555:LYS:HG3	2.04	0.57
5:F:82:ARG:O	5:F:86:HIS:HB2	2.03	0.57
3:N:996:TRP:CD2	3:N:1056:PRO:HG2	2.39	0.57
3:N:1324:PRO:HA	9:N:9374:HOH:O	2.02	0.57
5:P:118:GLU:HB3	9:P:7908:HOH:O	2.04	0.57
5:P:290:GLU:HG3	9:P:1848:HOH:O	2.05	0.57
3:N:65:ARG:HD3	3:N:66:GLN:H	1.70	0.57
3:N:1198:TYR:OH	3:N:1397:LYS:HE3	2.05	0.57
2:M:144:PRO:HB2	9:M:9612:HOH:O	2.04	0.57
3:D:467:GLU:HB2	9:D:9601:HOH:O	2.05	0.57
5:F:269:ASN:O	5:F:273:ARG:HG3	2.04	0.57
2:C:20:GLU:HG2	2:C:24:GLU:HG2	1.86	0.57
3:D:813:LEU:O	3:D:817:GLU:HB2	2.03	0.57
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.85	0.57
4:E:41:GLU:H	4:E:42:PRO:HD2	1.70	0.57
2:C:1025:ALA:HA	9:C:9926:HOH:O	2.04	0.57
2:M:984:GLU:HG2	3:N:944:THR:O	2.04	0.57
3:D:1490:LYS:HG3	9:D:9922:HOH:O	2.04	0.57
3:D:1239:ARG:HB2	9:D:3207:HOH:O	2.04	0.57
3:N:36:THR:HG22	3:N:38:LYS:HG3	1.87	0.57
2:C:70:GLU:HA	9:C:9597:HOH:O	2.03	0.57
5:P:79:ASP:O	5:P:83:GLN:HG3	2.04	0.57
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.39	0.57
2:M:964:LYS:O	2:M:968:LEU:HG	2.04	0.57
3:N:119:SER:CB	3:N:123:LEU:HB2	2.33	0.57
5:F:300:ASP:HA	9:F:9948:HOH:O	2.03	0.57
1:K:112:ARG:HD2	9:K:3292:HOH:O	2.03	0.57
4:E:54:LEU:HG	4:E:58:PRO:HD2	1.86	0.57
2:M:545:ASN:O	2:M:905:ILE:HD11	2.03	0.57
2:C:785:VAL:HG23	9:C:2281:HOH:O	2.04	0.57
3:N:925:GLU:HG2	9:O:1095:HOH:O	2.03	0.57
5:F:205:ARG:HG3	5:F:251:ILE:HD13	1.86	0.57
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.87	0.57
1:L:156:HIS:HD2	1:L:158:ILE:HG12	1.69	0.57
4:E:36:LYS:HD3	9:E:9576:HOH:O	2.04	0.57
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.86	0.57
1:A:212:ASN:O	1:A:215:VAL:HG22	2.05	0.57
2:M:642:ARG:HB3	9:M:9448:HOH:O	2.04	0.57
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.04	0.57
3:N:95:LEU:HD12	3:N:515:GLU:CA	2.34	0.57
2:M:165:LEU:HD21	2:M:334:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:677:MET:SD	2:C:987:ILE:HD13	2.44	0.57
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.33	0.57
5:P:416:ARG:HD2	5:P:419:ARG:CB	2.33	0.57
2:M:645:VAL:HG23	9:M:9422:HOH:O	2.05	0.57
5:F:366:ALA:O	5:F:370:LYS:HB3	2.04	0.57
3:D:999:THR:O	3:D:1002:LYS:HB2	2.05	0.57
3:D:194:GLY:H	3:D:206:ARG:HA	1.69	0.57
1:K:62:LEU:HD11	9:K:8889:HOH:O	2.04	0.57
2:M:524:VAL:HG22	2:M:525:SER:H	1.70	0.57
1:B:81:ASN:HB2	9:B:9809:HOH:O	2.03	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.40	0.57
1:A:10:VAL:HG21	9:A:9712:HOH:O	2.04	0.57
3:N:1250:ALA:HB3	9:N:9357:HOH:O	2.04	0.57
3:N:1164:ARG:HA	9:N:9915:HOH:O	2.04	0.57
3:N:179:VAL:HG21	9:N:2712:HOH:O	2.04	0.57
3:N:191:LEU:CB	3:N:195:VAL:HG21	2.30	0.57
3:D:642:CYS:SG	3:D:716:PHE:HB2	2.44	0.57
2:C:64:LEU:HD13	2:C:359:MET:SD	2.45	0.57
2:C:203:ASP:O	2:C:207:LEU:HB2	2.03	0.57
3:N:431:VAL:HG13	9:N:9967:HOH:O	2.05	0.57
5:F:288:TYR:HD2	5:F:304:VAL:HB	1.70	0.57
2:M:194:VAL:HG12	9:M:9819:HOH:O	2.04	0.57
2:C:417:GLY:O	2:C:418:LEU:HD13	2.05	0.57
3:D:966:GLU:HG2	3:D:970:LYS:HE2	1.87	0.57
2:C:495:THR:CG2	2:C:517:ARG:HE	2.15	0.57
3:N:1495:ILE:HD11	4:O:84:ARG:HE	1.69	0.57
2:C:538:GLN:HB2	9:C:2365:HOH:O	2.04	0.57
3:D:1119:SER:HB3	3:D:1185:GLU:HB3	1.85	0.57
3:N:701:LEU:HD21	3:N:763:MET:HE3	1.87	0.57
2:M:758:ARG:HB3	2:M:789:SER:HA	1.85	0.57
2:C:145:GLY:HA3	9:C:2144:HOH:O	2.04	0.57
2:C:163:ILE:HB	9:C:9761:HOH:O	2.05	0.57
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.04	0.57
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.86	0.57
3:D:1429:LEU:HG	9:D:2007:HOH:O	2.04	0.57
3:N:659:LYS:HG3	9:N:9809:HOH:O	2.02	0.57
4:E:15:SER:HB2	9:E:9581:HOH:O	2.05	0.57
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.04	0.57
3:N:1133:ARG:HD2	9:N:9227:HOH:O	2.04	0.57
3:D:83:SER:HA	9:D:9574:HOH:O	2.05	0.57
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:ALA:HA	2:C:218:VAL:CG2	2.35	0.57
2:M:66:LEU:HD11	2:M:98:LEU:HD22	1.87	0.57
3:D:871:LYS:HG3	3:D:873:LEU:HG	1.87	0.57
3:N:704:ARG:NH1	3:N:743:ASP:HB3	2.19	0.57
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.87	0.57
3:D:396:VAL:HG22	3:D:447:VAL:HB	1.87	0.57
1:K:62:LEU:H	1:K:62:LEU:HD12	1.70	0.57
3:D:32:ILE:O	5:F:258:ILE:HG23	2.03	0.57
3:N:584:ASN:H	3:N:602:SER:CB	2.18	0.57
1:A:211:LEU:O	1:A:215:VAL:HG13	2.03	0.57
3:N:25:GLU:HB3	9:N:9871:HOH:O	2.03	0.57
5:P:250:ALA:HB2	9:P:3340:HOH:O	2.04	0.57
3:D:1094:LEU:HB3	9:D:2067:HOH:O	2.05	0.57
5:P:194:LEU:HD22	9:P:1975:HOH:O	2.05	0.57
2:C:9:ILE:HG13	2:C:907:ASP:OD2	2.05	0.57
2:M:152:PRO:HA	9:M:2090:HOH:O	2.04	0.57
1:K:202:ASP:HA	9:K:1200:HOH:O	2.05	0.57
4:O:41:GLU:HB3	9:O:4432:HOH:O	2.04	0.57
3:D:192:ALA:O	3:D:195:VAL:HG23	2.04	0.57
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.20	0.57
5:F:316:SER:OG	5:F:318:GLU:HG3	2.04	0.57
2:M:737:LEU:HD11	2:M:754:ILE:HB	1.85	0.57
2:C:65:VAL:O	2:C:101:ILE:HG12	2.05	0.57
2:C:278:GLU:HG2	2:C:283:ILE:O	2.05	0.57
2:C:10:ARG:HG3	9:C:2815:HOH:O	2.04	0.57
3:D:799:LYS:HG2	3:D:826:PRO:HG2	1.86	0.57
2:M:1000:MET:HE3	2:M:1002:GLU:HB3	1.87	0.57
3:N:1031:ASN:HB3	3:N:1034:GLN:NE2	2.20	0.57
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.87	0.57
3:N:1096:ARG:HH11	3:N:1096:ARG:HB2	1.69	0.57
2:C:807:ARG:HG2	9:C:9967:HOH:O	2.05	0.57
2:M:226:VAL:HG12	9:M:2432:HOH:O	2.05	0.57
5:F:153:PRO:HB3	9:F:2137:HOH:O	2.05	0.57
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.19	0.57
5:P:74:LYS:HB2	9:P:2234:HOH:O	2.04	0.57
3:D:1390:LEU:HB2	9:D:2140:HOH:O	2.03	0.56
5:P:368:VAL:HA	9:P:5682:HOH:O	2.03	0.56
5:P:252:ALA:CB	5:P:265:VAL:HG21	2.30	0.56
2:M:1085:PHE:O	2:M:1088:LEU:HB3	2.05	0.56
2:M:545:ASN:ND2	2:M:905:ILE:HG13	2.19	0.56
3:D:834:THR:HB	3:D:838:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:183:SER:CB	2:M:190:LYS:HD3	2.34	0.56
2:C:250:ARG:HD3	9:C:9820:HOH:O	2.05	0.56
3:D:1503:VAL:HG11	9:D:2031:HOH:O	2.05	0.56
2:M:367:LEU:O	2:M:372:LEU:HD13	2.05	0.56
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.20	0.56
2:C:446:GLY:O	2:C:449:ILE:HG13	2.05	0.56
5:P:347:GLN:HB3	9:P:5652:HOH:O	2.04	0.56
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.87	0.56
4:O:44:GLU:O	4:O:45:ARG:HD3	2.04	0.56
3:N:423:ASP:OD2	5:P:174:LEU:HD22	2.05	0.56
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.86	0.56
2:M:490:GLU:HG2	2:M:494:TYR:CE1	2.40	0.56
1:L:83:LYS:HE2	1:L:167:VAL:HG12	1.86	0.56
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.85	0.56
4:O:32:ARG:HB2	4:O:32:ARG:HH11	1.70	0.56
1:A:141:GLU:HG3	9:A:9798:HOH:O	2.05	0.56
2:C:1009:SER:HB2	3:D:651:GLU:O	2.05	0.56
5:P:287:THR:HG22	5:P:290:GLU:OE1	2.05	0.56
3:D:701:LEU:C	3:D:702:LEU:HD12	2.25	0.56
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.87	0.56
3:N:984:THR:HG22	3:N:987:GLU:H	1.69	0.56
3:D:190:GLU:CD	3:D:190:GLU:H	2.09	0.56
2:M:1016:ILE:CD1	3:N:526:PRO:HG2	2.35	0.56
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.88	0.56
2:M:734:LEU:O	2:M:737:LEU:HB2	2.06	0.56
2:M:588:VAL:HG21	2:M:664:GLY:O	2.04	0.56
3:N:1348:LEU:O	3:N:1352:ILE:HG13	2.05	0.56
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.40	0.56
3:N:194:GLY:H	3:N:206:ARG:HA	1.70	0.56
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.40	0.56
3:D:1127:GLU:HB3	9:D:9585:HOH:O	2.04	0.56
3:N:1369:GLU:HB3	9:N:9676:HOH:O	2.06	0.56
1:B:162:ILE:HD13	9:B:9631:HOH:O	2.05	0.56
2:C:183:SER:OG	2:C:190:LYS:HD3	2.05	0.56
3:N:601:ARG:HH11	3:N:605:ASP:HB3	1.70	0.56
5:F:406:ARG:HG2	5:F:409:LYS:HD3	1.86	0.56
1:A:119:ASP:HB3	9:A:9566:HOH:O	2.05	0.56
3:N:1197:ARG:HB2	3:N:1396:GLU:OE2	2.04	0.56
9:C:9888:HOH:O	3:D:651:GLU:HB3	2.05	0.56
3:N:1203:LYS:HD3	9:N:9886:HOH:O	2.04	0.56
2:C:349:ALA:O	2:C:353:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:MET:SD	5:F:210:LEU:HB3	2.46	0.56
2:M:233:GLU:HG3	9:M:2295:HOH:O	2.04	0.56
2:C:866:PRO:HD2	9:C:9657:HOH:O	2.05	0.56
1:L:188:GLN:HA	9:L:1637:HOH:O	2.05	0.56
3:N:807:ALA:HB1	9:N:9607:HOH:O	2.06	0.56
2:M:2:GLU:HA	9:M:9520:HOH:O	2.05	0.56
3:N:379:ALA:HB2	9:N:2337:HOH:O	2.05	0.56
2:M:673:LEU:HB2	9:M:9318:HOH:O	2.04	0.56
5:P:262:VAL:HG23	9:P:3231:HOH:O	2.05	0.56
5:F:228:GLU:HA	9:F:9639:HOH:O	2.04	0.56
3:N:955:VAL:O	3:N:1039:CYS:HB3	2.06	0.56
2:C:420:ARG:HD2	9:C:2422:HOH:O	2.05	0.56
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.11	0.56
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.86	0.56
3:D:1332:PRO:HB2	9:D:9823:HOH:O	2.04	0.56
3:N:631:ILE:HG12	3:N:743:ASP:O	2.05	0.56
2:C:374:ASN:O	2:C:377:PRO:HD2	2.06	0.56
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.86	0.56
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.86	0.56
4:E:46:PRO:HD2	9:E:9659:HOH:O	2.04	0.56
2:M:723:THR:C	2:M:725:ASP:H	2.09	0.56
2:C:185:LYS:HD3	2:C:190:LYS:HE2	1.86	0.56
1:K:151:VAL:HB	1:K:169:ALA:HB3	1.86	0.56
2:C:804:VAL:HG11	9:C:2137:HOH:O	2.05	0.56
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.87	0.56
3:D:820:GLU:HA	3:D:825:ALA:O	2.04	0.56
2:C:1108:PRO:HG3	9:C:9868:HOH:O	2.05	0.56
3:N:148:GLU:HA	9:N:9837:HOH:O	2.04	0.56
3:N:169:TYR:N	3:N:170:PRO:HD3	2.20	0.56
3:N:172:PRO:HA	3:N:178:LEU:HD13	1.88	0.56
3:N:169:TYR:HA	3:N:392:SER:HA	1.87	0.56
3:N:12:LEU:HD23	3:N:13:ALA:H	1.70	0.56
3:D:168:THR:CB	3:D:393:ILE:HD12	2.36	0.56
5:P:160:ASP:O	5:P:163:LEU:HB2	2.05	0.56
3:N:834:THR:HA	3:N:838:ARG:HH21	1.70	0.56
5:F:413:SER:HA	5:F:416:ARG:CZ	2.36	0.56
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.05	0.56
2:C:859:PRO:O	2:C:867:VAL:HG22	2.05	0.56
2:C:861:LEU:HD23	2:C:862:PRO:N	2.21	0.56
5:F:80:PRO:HG2	9:F:9637:HOH:O	2.04	0.56
1:A:123:MET:C	1:A:125:PRO:HD3	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:ILE:H	3:D:141:ILE:HD12	1.69	0.56
3:N:999:THR:O	3:N:1002:LYS:HB2	2.06	0.56
3:N:681:ARG:HB2	3:N:681:ARG:NH1	2.20	0.56
3:N:221:ALA:HA	9:N:9249:HOH:O	2.04	0.56
3:D:1437:ALA:O	3:D:1446:VAL:HG21	2.05	0.56
3:N:430:ASP:HB2	3:N:432:TYR:CE2	2.41	0.56
2:M:696:LYS:HA	9:M:9221:HOH:O	2.06	0.56
1:K:70:GLY:HA2	1:K:133:GLU:HG2	1.87	0.56
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.87	0.56
2:M:710:ILE:HB	2:M:790:LEU:HD22	1.86	0.56
3:D:447:VAL:HG22	9:D:9908:HOH:O	2.05	0.56
5:F:92:PRO:HB3	9:F:9758:HOH:O	2.05	0.56
2:M:292:ARG:HB2	2:M:299:LYS:HZ2	1.71	0.56
3:D:893:GLU:HB2	9:D:2572:HOH:O	2.06	0.56
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.87	0.56
1:L:18:ARG:O	1:L:207:PRO:HD3	2.06	0.56
3:D:1087:ARG:NH1	3:D:1234:THR:HA	2.21	0.56
3:D:64:LYS:HD3	9:F:9603:HOH:O	2.04	0.56
1:A:188:GLN:HG3	1:A:189:ARG:H	1.71	0.56
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.87	0.56
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.05	0.56
5:P:135:ILE:HD11	5:P:178:ARG:HB3	1.88	0.56
3:N:877:PRO:O	3:N:880:ILE:HG22	2.05	0.56
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.36	0.56
2:C:101:ILE:HG22	2:C:102:HIS:H	1.71	0.56
2:C:367:LEU:O	2:C:372:LEU:HD13	2.06	0.56
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.05	0.56
4:E:44:GLU:HA	9:E:9565:HOH:O	2.04	0.56
2:M:760:SER:O	2:M:785:VAL:HG22	2.05	0.56
3:N:1433:SER:HB2	3:N:1457:ASP:OD2	2.06	0.56
5:P:120:THR:HB	5:P:122:LEU:HB2	1.88	0.56
5:F:102:LEU:O	5:F:106:VAL:HG23	2.06	0.56
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.88	0.56
2:M:654:LEU:HD21	2:M:663:ASN:ND2	2.21	0.56
3:D:828:LYS:HD3	3:D:828:LYS:N	2.20	0.56
2:M:889:HIS:NE2	2:M:970:GLY:HA3	2.21	0.56
3:N:86:ARG:O	3:N:522:PRO:HD2	2.06	0.56
5:P:267:THR:HG23	5:P:299:TRP:HH2	1.70	0.56
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.06	0.56
1:K:63:HIS:HA	9:K:1147:HOH:O	2.06	0.56
2:C:208:ALA:HA	2:C:218:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:LEU:O	3:D:120:ALA:N	2.39	0.56
3:D:123:LEU:HA	9:D:2113:HOH:O	2.06	0.56
3:N:1045:MET:CG	3:N:1073:SER:HA	2.33	0.56
2:M:237:ARG:HG2	9:M:9833:HOH:O	2.05	0.56
3:D:1137:ARG:H	3:D:1137:ARG:CD	2.18	0.56
3:D:1379:VAL:HG22	9:D:2424:HOH:O	2.05	0.56
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.41	0.56
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.88	0.56
3:D:131:LYS:HB3	3:D:568:ARG:HG2	1.87	0.56
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.41	0.56
1:K:73:GLU:HG3	1:K:130:ALA:HA	1.88	0.56
2:M:56:GLU:HB3	9:M:9316:HOH:O	2.06	0.56
3:N:553:ARG:HA	3:N:556:LYS:HD3	1.86	0.56
2:M:117:HIS:HB2	9:M:9333:HOH:O	2.05	0.56
4:O:7:ASP:HB2	9:O:4398:HOH:O	2.05	0.56
2:M:674:VAL:HG12	2:M:990:GLY:O	2.06	0.56
2:C:244:PRO:CD	2:C:245:GLY:H	2.16	0.56
5:P:151:LEU:HB3	9:P:4293:HOH:O	2.05	0.56
4:E:48:MET:HG2	4:E:49:GLN:H	1.70	0.56
2:M:14:PRO:HA	9:M:9656:HOH:O	2.06	0.56
5:P:141:VAL:HB	9:P:2295:HOH:O	2.06	0.56
3:N:1294:VAL:HB	9:N:9684:HOH:O	2.04	0.56
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.87	0.56
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.40	0.56
2:C:63:GLY:HA3	2:C:103:LYS:HG2	1.88	0.56
2:M:573:ARG:HB3	2:M:670:GLN:NE2	2.20	0.56
2:C:44:ILE:HA	9:C:9646:HOH:O	2.05	0.56
2:C:47:ALA:HA	9:C:9778:HOH:O	2.05	0.56
3:D:36:THR:C	3:D:38:LYS:H	2.09	0.56
5:P:205:ARG:HG3	5:P:251:ILE:HD13	1.87	0.56
2:M:261:ILE:HG22	2:M:262:ALA:H	1.71	0.56
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.21	0.56
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.87	0.56
3:D:496:LEU:HD11	3:D:500:ARG:HE	1.70	0.56
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.36	0.56
2:C:742:VAL:HG21	9:C:9683:HOH:O	2.06	0.56
5:F:287:THR:HG22	5:F:290:GLU:OE1	2.06	0.56
2:C:734:LEU:O	2:C:737:LEU:HB2	2.06	0.56
3:N:709:HIS:CD2	3:N:1231:GLU:HG3	2.41	0.56
3:D:1314:LYS:HD3	3:D:1314:LYS:N	2.21	0.56
2:C:247:PRO:HD2	9:C:9820:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1150:ALA:HA	9:D:9851:HOH:O	2.06	0.56
1:K:41:ARG:HG3	1:K:177:VAL:HB	1.88	0.56
3:D:728:LEU:HD22	3:D:745:MET:SD	2.45	0.56
3:N:1462:LEU:HD21	3:N:1474:ALA:HB2	1.88	0.56
1:K:88:ARG:NH1	1:K:90:LEU:HD23	2.21	0.56
2:M:881:ASN:ND2	2:M:881:ASN:H	2.03	0.56
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.06	0.56
1:K:192:LEU:HD21	9:K:1294:HOH:O	2.06	0.56
2:M:770:GLU:HB3	5:P:350:LEU:HD21	1.88	0.56
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.88	0.56
5:P:124:PRO:HB3	9:P:1676:HOH:O	2.06	0.56
2:C:99:GLN:HB3	2:C:109:LYS:HG3	1.87	0.56
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.87	0.55
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.32	0.55
3:N:22:SER:HA	3:N:90:MET:O	2.06	0.55
4:O:47:LYS:N	4:O:54:LEU:HD22	2.22	0.55
2:M:398:THR:HA	2:M:633:GLN:HG3	1.88	0.55
1:L:123:MET:C	1:L:125:PRO:HD3	2.26	0.55
3:N:390:PRO:HG2	5:P:98:GLU:OE1	2.06	0.55
2:C:831:ARG:HA	9:C:9680:HOH:O	2.06	0.55
3:D:12:LEU:HD21	3:D:104:PHE:HE1	1.71	0.55
3:D:1065:LEU:HD12	3:D:1069:GLU:HB3	1.88	0.55
3:D:207:PHE:HA	9:D:3106:HOH:O	2.05	0.55
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.87	0.55
4:O:32:ARG:NH1	4:O:32:ARG:HB2	2.20	0.55
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.88	0.55
3:N:456:MET:SD	3:N:568:ARG:HD3	2.46	0.55
2:M:369:PRO:HB3	9:M:2382:HOH:O	2.07	0.55
3:N:1029:ARG:CZ	8:N:9101:G4P:O2D	2.54	0.55
2:M:492:ASP:HB3	2:M:518:LYS:HD2	1.87	0.55
2:C:536:PRO:HD2	2:C:537:LYS:HZ3	1.71	0.55
2:C:890:LEU:HD13	2:C:914:ILE:HG13	1.88	0.55
1:A:115:LEU:HB3	9:A:9587:HOH:O	2.06	0.55
5:P:197:SER:HB2	9:P:5517:HOH:O	2.06	0.55
3:D:400:VAL:HA	3:D:442:ASN:O	2.06	0.55
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.70	0.55
3:D:1473:PRO:HB2	9:D:3112:HOH:O	2.05	0.55
1:L:177:VAL:HG13	1:L:197:LEU:HD21	1.88	0.55
3:N:1008:PHE:O	3:N:1012:GLU:HG3	2.06	0.55
4:E:45:ARG:HB3	4:E:46:PRO:HD2	1.89	0.55
3:N:703:ASN:HD22	3:N:713:ILE:HG12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:361:LEU:HD21	5:F:408:LEU:HD12	1.88	0.55
3:N:477:LEU:HD23	9:N:2072:HOH:O	2.06	0.55
3:N:166:GLN:HB3	3:N:395:VAL:HG21	1.87	0.55
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.41	0.55
9:N:2002:HOH:O	5:P:315:VAL:HG11	2.06	0.55
2:M:670:GLN:HE22	2:M:699:PHE:HA	1.71	0.55
1:B:170:VAL:HG22	9:B:9562:HOH:O	2.05	0.55
2:M:553:ASP:HA	2:M:881:ASN:HA	1.88	0.55
2:M:482:GLU:HB3	9:M:9208:HOH:O	2.06	0.55
2:M:191:PHE:HA	9:M:9556:HOH:O	2.06	0.55
3:N:1390:LEU:HD22	9:N:9553:HOH:O	2.06	0.55
3:N:1372:VAL:HA	3:N:1375:MET:CE	2.36	0.55
2:C:614:ARG:HD2	9:C:2802:HOH:O	2.07	0.55
2:M:768:THR:HG22	2:M:771:GLU:H	1.72	0.55
3:N:964:LEU:HG	9:N:9387:HOH:O	2.06	0.55
9:K:1228:HOH:O	2:M:856:GLU:HB3	2.06	0.55
3:D:908:LYS:HB3	3:D:1027:GLY:CA	2.27	0.55
3:D:423:ASP:OD2	5:F:174:LEU:HD22	2.07	0.55
3:N:1137:ARG:HA	9:N:9839:HOH:O	2.06	0.55
2:C:139:GLN:NE2	2:C:415:PRO:HD2	2.17	0.55
5:F:115:LYS:HE3	9:F:9566:HOH:O	2.07	0.55
2:C:949:LYS:HD2	3:D:796:ARG:NH2	2.21	0.55
5:P:161:GLN:HG2	9:P:1559:HOH:O	2.06	0.55
1:B:175:ARG:O	3:D:851:LEU:HD21	2.07	0.55
1:A:223:THR:HG22	9:A:9752:HOH:O	2.05	0.55
2:C:503:LEU:HD12	2:C:507:ARG:O	2.06	0.55
3:D:644:LEU:HG	3:D:718:PRO:HB3	1.89	0.55
2:M:250:ARG:HE	2:M:253:ALA:CB	2.19	0.55
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.41	0.55
5:P:81:VAL:HG23	9:P:1606:HOH:O	2.04	0.55
3:N:1119:SER:HB2	3:N:1185:GLU:HB3	1.87	0.55
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.87	0.55
3:N:625:TYR:O	3:N:749:VAL:HG23	2.07	0.55
2:M:841:ASN:H	2:M:841:ASN:HD22	1.55	0.55
5:F:166:LEU:O	5:F:171:LYS:HB2	2.06	0.55
3:D:775:GLY:HA3	3:D:1145:TYR:CE1	2.37	0.55
5:F:320:PRO:O	5:F:321:ILE:HD13	2.07	0.55
2:M:3:ILE:HG22	9:M:9511:HOH:O	2.05	0.55
3:N:1497:GLU:O	3:N:1501:GLU:HG3	2.07	0.55
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.87	0.55
3:N:613:ARG:HD2	9:N:2236:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:ILE:HG23	9:D:9965:HOH:O	2.06	0.55
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.89	0.55
3:N:36:THR:C	3:N:38:LYS:H	2.09	0.55
4:E:90:GLU:HB2	9:E:9648:HOH:O	2.05	0.55
3:D:165:LYS:HD3	3:D:165:LYS:O	2.06	0.55
2:C:57:GLU:O	2:C:62:GLY:HA3	2.06	0.55
3:N:1449:GLU:O	3:N:1452:ILE:HG22	2.07	0.55
5:F:280:GLN:HG2	5:F:281:GLU:HG3	1.89	0.55
5:P:85:LEU:HD13	9:P:5383:HOH:O	2.05	0.55
2:C:328:LEU:HD21	2:C:434:HIS:HD2	1.71	0.55
2:M:516:ARG:NH1	3:N:1068:LEU:HD22	2.21	0.55
2:C:333:ILE:HD13	2:C:467:ILE:HD11	1.87	0.55
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.21	0.55
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.07	0.55
1:K:86:VAL:HG13	1:K:123:MET:HB2	1.89	0.55
1:K:49:PRO:HA	1:K:148:VAL:HG12	1.89	0.55
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.88	0.55
2:M:524:VAL:CG2	2:M:528:GLU:HB2	2.36	0.55
5:F:143:HIS:HB3	9:F:9613:HOH:O	2.05	0.55
3:D:539:ASP:HA	9:D:2979:HOH:O	2.06	0.55
3:D:93:ILE:HG22	9:D:2002:HOH:O	2.07	0.55
2:C:577:PRO:HG3	2:C:993:PHE:CZ	2.42	0.55
3:D:710:ARG:HG3	3:D:711:LEU:HD22	1.89	0.55
3:D:1389:LEU:HD23	3:D:1389:LEU:H	1.72	0.55
4:O:31:LEU:HD21	4:O:60:ALA:CB	2.36	0.55
4:O:42:PRO:HD2	9:O:4230:HOH:O	2.05	0.55
5:P:363:GLU:HG2	5:P:364:ARG:N	2.22	0.55
5:F:278:LEU:HB3	5:F:286:PRO:CG	2.31	0.55
2:M:777:ILE:HG13	5:P:405:LEU:HD11	1.88	0.55
2:M:417:GLY:O	2:M:418:LEU:HD13	2.06	0.55
3:D:126:VAL:HG11	9:D:2381:HOH:O	2.05	0.55
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.72	0.55
2:M:218:VAL:HG13	9:M:9323:HOH:O	2.07	0.55
2:C:290:LEU:HB3	9:C:9841:HOH:O	2.05	0.55
2:M:1043:TYR:CE2	3:N:763:MET:HA	2.42	0.55
2:C:227:PHE:HB3	9:C:2116:HOH:O	2.07	0.55
2:C:254:VAL:HG22	2:C:258:TYR:CE1	2.42	0.55
3:D:39:PRO:HB3	3:D:45:PHE:C	2.26	0.55
1:B:99:LEU:HA	9:B:9656:HOH:O	2.06	0.55
2:M:226:VAL:HG21	9:M:2143:HOH:O	2.05	0.55
2:M:275:TYR:O	2:M:279:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:HIS:HA	3:D:519:VAL:HG23	1.87	0.55
1:L:214:ALA:HA	1:L:217:ILE:HD12	1.88	0.55
3:N:758:GLU:HB3	4:O:20:THR:HG21	1.88	0.55
3:D:1118:ILE:HD11	3:D:1192:LEU:HB2	1.89	0.55
3:D:485:SER:HB2	9:D:3145:HOH:O	2.05	0.55
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.89	0.55
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.87	0.55
3:D:138:LYS:HG3	9:D:2920:HOH:O	2.05	0.55
3:N:141:ILE:HG21	9:N:9453:HOH:O	2.06	0.55
3:N:1243:THR:HB	3:N:1253:THR:HB	1.88	0.55
2:C:367:LEU:HA	2:C:371:LYS:HB2	1.89	0.55
2:C:492:ASP:HB2	9:C:2376:HOH:O	2.06	0.55
1:K:158:ILE:HB	9:K:2046:HOH:O	2.05	0.55
1:B:7:LYS:O	1:B:7:LYS:HD2	2.07	0.55
3:D:645:PRO:HA	3:D:721:VAL:O	2.07	0.55
3:N:149:LYS:HD3	3:N:149:LYS:H	1.71	0.55
3:N:36:THR:HG22	9:N:9685:HOH:O	2.06	0.55
2:C:444:PRO:HA	9:C:9645:HOH:O	2.06	0.55
2:M:57:GLU:O	2:M:62:GLY:HA3	2.06	0.55
3:N:787:LEU:HD21	3:N:947:ILE:HD13	1.88	0.55
1:K:42:ARG:HD2	9:K:4396:HOH:O	2.07	0.55
3:D:1101:VAL:HG11	3:D:1427:SER:HB3	1.88	0.55
3:D:1468:LEU:HD21	9:D:2087:HOH:O	2.07	0.55
2:M:720:GLU:HG2	9:M:9228:HOH:O	2.07	0.55
5:P:170:HIS:HA	5:P:173:TYR:CD1	2.41	0.55
1:A:104:GLU:HB2	9:A:9584:HOH:O	2.06	0.55
1:L:48:ILE:HG22	1:L:173:PRO:HD2	1.88	0.55
3:N:107:ASP:OD2	3:N:109:PRO:HD2	2.07	0.55
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.21	0.55
5:F:136:LEU:HD11	5:F:141:VAL:HG21	1.89	0.55
1:K:27:PRO:HB2	9:K:1056:HOH:O	2.06	0.55
3:D:1365:ASP:O	3:D:1369:GLU:HG3	2.07	0.55
5:F:153:PRO:HG2	5:F:154:LYS:H	1.71	0.55
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.06	0.55
3:D:543:LEU:HA	3:D:546:ARG:HG2	1.89	0.55
3:N:1496:GLU:HB2	9:N:9255:HOH:O	2.05	0.55
5:P:196:VAL:O	5:P:200:LYS:HB2	2.07	0.55
2:M:323:ASP:HA	9:M:9235:HOH:O	2.06	0.55
2:C:405:ARG:HD3	2:C:543:ASN:ND2	2.22	0.55
2:C:755:LEU:CD1	2:C:825:VAL:HG11	2.34	0.55
1:B:23:PHE:CZ	1:B:208:LEU:HD22	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:534:VAL:H	2:M:538:GLN:HE22	1.55	0.55
1:L:41:ARG:NH1	1:L:177:VAL:HB	2.21	0.55
3:D:812:ALA:HA	9:D:9733:HOH:O	2.06	0.55
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.87	0.55
1:A:178:ALA:CB	2:C:864:GLY:H	2.20	0.55
1:K:60:ASP:HB3	9:K:4731:HOH:O	2.06	0.55
3:D:1442:ASN:HB3	9:D:3067:HOH:O	2.06	0.55
2:M:614:ARG:HD3	9:M:9224:HOH:O	2.05	0.55
3:D:554:LEU:HG	9:D:9809:HOH:O	2.06	0.55
2:C:589:ARG:HD3	2:C:596:TYR:CE2	2.41	0.55
4:E:84:ARG:HD2	4:E:87:LYS:HD3	1.89	0.55
2:M:1105:LYS:HG2	9:M:9543:HOH:O	2.07	0.55
1:K:146:ARG:HG3	9:K:1164:HOH:O	2.06	0.55
2:M:944:LEU:O	2:M:947:ALA:HB3	2.07	0.55
3:D:53:ILE:HG22	9:D:2190:HOH:O	2.07	0.55
3:D:133:ILE:HG12	9:D:9996:HOH:O	2.06	0.54
3:N:177:ALA:CA	3:N:199:LEU:HD13	2.38	0.54
3:D:1487:VAL:HG23	4:E:74:VAL:O	2.07	0.54
2:M:567:GLN:HE22	2:M:838:LYS:NZ	2.05	0.54
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.41	0.54
3:D:729:HIS:CE1	3:D:731:LEU:HG	2.42	0.54
3:N:596:SER:HA	9:N:2771:HOH:O	2.08	0.54
3:N:1119:SER:HA	3:N:1186:VAL:O	2.07	0.54
3:N:1124:GLN:CD	3:N:1135:ARG:HA	2.28	0.54
5:P:125:ASP:O	5:P:129:GLU:HG2	2.07	0.54
1:K:76:VAL:HA	1:K:79:ILE:HG12	1.89	0.54
3:D:1468:LEU:HD23	3:D:1468:LEU:O	2.07	0.54
3:D:1481:VAL:CG1	4:E:18:ARG:HA	2.34	0.54
3:N:648:MET:HG2	3:N:652:LEU:HD23	1.88	0.54
4:E:57:ASP:H	4:E:58:PRO:HD3	1.73	0.54
5:F:371:LEU:HD11	9:F:9735:HOH:O	2.07	0.54
3:D:487:ALA:HB1	3:D:488:ARG:HH21	1.71	0.54
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.37	0.54
5:F:93:LEU:HG	5:F:190:ALA:CB	2.37	0.54
5:P:323:ASP:HB3	9:P:4379:HOH:O	2.07	0.54
2:M:376:ARG:HB3	2:M:377:PRO:HD3	1.88	0.54
2:M:108:ILE:HG12	9:M:2211:HOH:O	2.06	0.54
5:F:302:LYS:HA	9:F:9730:HOH:O	2.06	0.54
3:D:470:LEU:HB2	3:D:503:LEU:HD21	1.89	0.54
2:C:111:ASP:HA	9:C:2107:HOH:O	2.06	0.54
1:B:135:GLY:HA3	9:B:9591:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:197:SER:CB	3:D:203:ALA:HB3	2.30	0.54
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.37	0.54
2:M:1051:GLU:C	2:M:1056:LYS:HD2	2.28	0.54
2:M:1057:SER:OG	3:N:621:LYS:HE2	2.07	0.54
2:C:1013:TYR:HB3	9:C:2050:HOH:O	2.06	0.54
3:N:704:ARG:HD2	3:N:705:ALA:H	1.71	0.54
3:D:146:PRO:HG2	9:D:9704:HOH:O	2.07	0.54
5:P:166:LEU:O	5:P:171:LYS:HB2	2.07	0.54
5:F:181:GLU:O	5:F:184:ARG:HB3	2.08	0.54
2:M:719:PRO:HD3	9:M:2003:HOH:O	2.07	0.54
2:C:897:LEU:HD11	2:C:920:GLN:HG3	1.89	0.54
2:C:1081:VAL:HB	2:C:1086:ARG:NE	2.22	0.54
3:D:19:ARG:HA	9:D:2218:HOH:O	2.07	0.54
5:F:262:VAL:HG23	9:F:9614:HOH:O	2.07	0.54
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.07	0.54
4:E:56:ASP:HB2	9:E:9649:HOH:O	2.07	0.54
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.90	0.54
2:M:532:MET:HE1	9:M:9849:HOH:O	2.06	0.54
2:C:165:LEU:HD13	9:C:2088:HOH:O	2.06	0.54
2:M:159:ILE:HB	9:M:9671:HOH:O	2.06	0.54
3:D:816:HIS:HA	9:D:3219:HOH:O	2.07	0.54
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.88	0.54
3:D:41:ARG:HG3	9:D:9655:HOH:O	2.05	0.54
1:B:137:ARG:NH1	1:B:139:ASN:HB3	2.21	0.54
3:D:1169:ASP:HB2	9:D:2059:HOH:O	2.07	0.54
1:A:62:LEU:HD12	1:A:62:LEU:H	1.71	0.54
3:D:1449:GLU:HB2	9:D:9628:HOH:O	2.07	0.54
1:K:206:THR:HG22	1:K:209:GLU:HG3	1.88	0.54
1:A:7:LYS:NZ	1:A:186:LEU:HD23	2.22	0.54
2:C:328:LEU:CD1	2:C:433:THR:HB	2.26	0.54
5:P:367:MET:HB3	5:P:370:LYS:HZ2	1.72	0.54
2:M:1089:VAL:O	2:M:1093:GLN:HG2	2.07	0.54
2:M:649:VAL:HA	2:M:650:ARG:NH2	2.22	0.54
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.89	0.54
2:M:159:ILE:HG21	2:M:175:GLU:OE1	2.07	0.54
3:N:634:GLY:O	3:N:637:LEU:HB3	2.07	0.54
3:N:693:GLU:HA	9:N:9838:HOH:O	2.05	0.54
2:C:666:LEU:HD12	2:C:667:ALA:H	1.73	0.54
3:N:838:ARG:HD2	3:N:874:GLU:OE2	2.08	0.54
2:C:1015:LEU:HB3	2:C:1016:ILE:HD13	1.88	0.54
3:N:814:ALA:HB2	9:N:9382:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:400:VAL:HG23	9:N:2141:HOH:O	2.07	0.54
1:K:18:ARG:NH2	1:K:88:ARG:HH21	2.05	0.54
2:M:286:SER:HB3	2:M:299:LYS:HE2	1.89	0.54
1:A:186:LEU:HB2	9:A:9592:HOH:O	2.07	0.54
3:N:638:LYS:HE2	9:N:2726:HOH:O	2.08	0.54
2:C:455:LEU:HD13	2:C:456:ALA:O	2.07	0.54
9:K:6214:HOH:O	1:L:229:GLN:HB3	2.06	0.54
2:M:72:ARG:HB3	9:M:9754:HOH:O	2.07	0.54
3:N:101:HIS:O	3:N:105:VAL:HG23	2.07	0.54
2:C:598:GLU:O	2:C:651:LYS:HG3	2.07	0.54
2:C:640:ARG:HD3	2:C:642:ARG:NH2	2.22	0.54
3:D:1209:LEU:CD2	3:D:1216:SER:H	2.21	0.54
1:L:9:PRO:HD3	9:L:3141:HOH:O	2.07	0.54
5:F:314:PRO:HD3	9:F:9825:HOH:O	2.07	0.54
1:A:41:ARG:HG3	1:A:177:VAL:HB	1.88	0.54
3:D:1033:GLN:HB3	3:D:1036:ARG:HH21	1.73	0.54
3:N:100:ALA:H	3:N:575:GLN:HE22	1.54	0.54
1:K:189:ARG:HD2	9:K:1183:HOH:O	2.08	0.54
3:D:608:SER:O	3:D:614:PHE:HB2	2.08	0.54
5:F:364:ARG:HH11	5:F:364:ARG:HB3	1.72	0.54
2:C:53:PRO:HA	9:C:9804:HOH:O	2.07	0.54
4:O:60:ALA:O	4:O:63:TRP:HB2	2.08	0.54
2:M:34:VAL:HG22	9:M:9591:HOH:O	2.07	0.54
1:L:80:LEU:CD1	3:N:842:VAL:HG12	2.35	0.54
3:D:1397:LYS:HG3	9:D:2561:HOH:O	2.08	0.54
4:E:47:LYS:N	4:E:54:LEU:HD22	2.23	0.54
3:N:138:LYS:H	3:N:138:LYS:HD2	1.73	0.54
1:B:94:LEU:HD21	1:B:119:ASP:OD1	2.08	0.54
3:N:1408:ILE:HB	9:N:9535:HOH:O	2.07	0.54
1:L:143:ARG:HE	1:L:158:ILE:HG21	1.72	0.54
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.54
5:F:153:PRO:HB2	9:F:9865:HOH:O	2.07	0.54
2:M:2:GLU:HB3	9:M:2027:HOH:O	2.07	0.54
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.90	0.54
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.90	0.54
2:M:495:THR:HA	9:M:9319:HOH:O	2.08	0.54
3:D:669:ASN:HD21	3:D:671:LYS:HB2	1.72	0.54
3:N:246:PRO:HA	9:N:2931:HOH:O	2.06	0.54
2:C:1054:THR:HG23	2:C:1059:ASP:HB2	1.90	0.54
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.89	0.54
3:D:637:LEU:HD11	3:D:642:CYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:266:ARG:HB3	9:M:9251:HOH:O	2.06	0.54
2:M:208:ALA:HB2	9:M:9323:HOH:O	2.08	0.54
3:D:761:ILE:HD11	4:E:23:VAL:HG11	1.89	0.54
2:M:469:THR:N	9:M:9590:HOH:O	2.40	0.54
1:B:41:ARG:NH1	1:B:177:VAL:HB	2.22	0.54
1:A:88:ARG:HB2	1:A:204:SER:HA	1.90	0.54
9:M:9528:HOH:O	5:P:280:GLN:HA	2.07	0.54
3:N:149:LYS:N	3:N:149:LYS:HD3	2.23	0.54
2:M:279:GLU:HG3	2:M:280:LYS:HG3	1.89	0.54
4:O:14:ASP:HA	9:O:5443:HOH:O	2.08	0.54
2:M:383:ARG:HG3	9:M:9744:HOH:O	2.07	0.54
2:C:105:THR:HG23	9:C:9938:HOH:O	2.07	0.54
3:D:441:ARG:HB3	3:D:443:VAL:CG2	2.37	0.54
1:B:107:LYS:HB3	9:B:9616:HOH:O	2.08	0.54
4:E:69:LEU:HD11	9:E:9579:HOH:O	2.07	0.54
3:D:1258:ARG:HG2	3:D:1262:LEU:HD13	1.89	0.54
3:D:474:GLU:HG3	3:D:500:ARG:HE	1.72	0.54
2:C:405:ARG:HH12	2:C:409:ARG:NH2	2.00	0.54
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.32	0.54
2:M:1093:GLN:NE2	2:M:1099:VAL:H	2.06	0.54
2:C:1014:SER:HB2	5:F:331:ASP:HA	1.90	0.54
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.89	0.54
3:D:1119:SER:HA	3:D:1186:VAL:O	2.08	0.54
3:N:537:THR:O	5:P:317:LEU:HB2	2.08	0.54
2:C:45:GLN:HG2	9:C:9991:HOH:O	2.07	0.54
1:B:74:ASP:HA	9:B:9649:HOH:O	2.07	0.54
5:F:89:GLY:HA3	9:F:9884:HOH:O	2.08	0.54
2:M:425:PHE:HB3	9:N:9251:HOH:O	2.07	0.54
2:M:346:VAL:O	2:M:350:ARG:HG3	2.08	0.54
2:C:798:GLY:H	2:C:827:VAL:CG1	2.20	0.54
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.08	0.54
3:D:1312:LEU:HA	9:D:3003:HOH:O	2.08	0.54
3:D:404:GLU:HB3	3:D:414:ARG:NE	2.23	0.54
3:D:1462:LEU:HD21	3:D:1474:ALA:HB2	1.89	0.54
2:C:305:PRO:O	2:C:308:ARG:HB3	2.07	0.54
3:N:523:ASP:N	9:N:9625:HOH:O	2.41	0.54
3:N:644:LEU:HD12	3:N:645:PRO:N	2.23	0.54
3:D:141:ILE:HG12	3:D:449:SER:HA	1.89	0.54
5:P:270:LYS:HD2	9:P:8061:HOH:O	2.08	0.54
5:F:158:GLU:O	5:F:161:GLN:HB2	2.07	0.54
1:B:73:GLU:HG3	1:B:130:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:140:ARG:HA	9:F:9613:HOH:O	2.08	0.54
1:A:119:ASP:HA	9:A:9646:HOH:O	2.07	0.54
2:C:714:ASP:OD2	2:C:719:PRO:HG3	2.08	0.54
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.89	0.54
2:M:320:HIS:HA	9:M:9779:HOH:O	2.08	0.54
3:D:62:LYS:HG3	9:D:2359:HOH:O	2.07	0.54
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.07	0.54
2:M:637:LEU:HD23	2:M:659:PRO:HG2	1.89	0.54
2:M:448:ASN:HB2	2:M:452:ILE:HD11	1.89	0.54
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.38	0.53
2:C:356:ARG:HA	9:C:2205:HOH:O	2.07	0.53
2:M:266:ARG:HB2	2:M:288:ARG:NH1	2.23	0.53
2:M:50:GLU:HB3	9:M:9948:HOH:O	2.07	0.53
2:C:944:LEU:O	2:C:947:ALA:HB3	2.08	0.53
2:C:1019:GLN:HE21	3:D:621:LYS:HG3	1.73	0.53
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.38	0.53
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.90	0.53
1:L:86:VAL:HG13	1:L:123:MET:HB2	1.89	0.53
2:C:535:SER:OG	2:C:537:LYS:HE2	2.08	0.53
3:D:935:LYS:NZ	3:D:935:LYS:HB3	2.23	0.53
1:A:86:VAL:HG13	1:A:123:MET:HB2	1.90	0.53
5:P:291:ILE:HD13	5:P:304:VAL:CG1	2.38	0.53
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.89	0.53
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.90	0.53
3:D:546:ARG:O	3:D:550:ARG:HG2	2.08	0.53
9:M:9380:HOH:O	5:P:279:GLN:HG2	2.09	0.53
5:P:222:ARG:HD3	9:P:1708:HOH:O	2.08	0.53
3:N:190:GLU:CD	3:N:190:GLU:H	2.11	0.53
2:M:916:GLU:HA	9:M:9478:HOH:O	2.07	0.53
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	2.08	0.53
3:N:389:GLU:HG3	9:N:2712:HOH:O	2.08	0.53
2:M:148:PHE:HB3	2:M:313:LEU:CD2	2.36	0.53
2:M:368:THR:HB	2:M:369:PRO:HD3	1.90	0.53
2:C:31:GLN:HG3	2:C:40:GLU:O	2.08	0.53
2:M:173:ASP:HB2	2:M:185:LYS:HE3	1.89	0.53
3:D:720:LEU:H	3:D:720:LEU:HD12	1.71	0.53
3:N:99:ALA:HB1	3:N:575:GLN:NE2	2.23	0.53
2:C:408:ARG:NH1	2:C:542:VAL:HG13	2.23	0.53
2:M:244:PRO:HB3	9:M:9820:HOH:O	2.08	0.53
2:M:253:ALA:O	2:M:256:TYR:HB2	2.08	0.53
5:F:277:GLN:O	5:F:280:GLN:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.90	0.53
3:N:96:ALA:HB3	3:N:554:LEU:HG	1.90	0.53
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.90	0.53
3:D:1009:LYS:HE3	9:D:2148:HOH:O	2.09	0.53
2:C:84:ARG:HH12	2:C:128:ILE:HD13	1.73	0.53
3:N:1063:GLU:HG3	3:N:1064:GLY:H	1.72	0.53
3:N:1066:THR:HG23	3:N:1069:GLU:OE1	2.08	0.53
9:A:9633:HOH:O	2:C:607:ASP:HA	2.08	0.53
9:N:9959:HOH:O	5:P:375:LEU:HD13	2.08	0.53
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.29	0.53
3:N:486:ARG:O	3:N:489:ARG:HG2	2.08	0.53
5:F:292:ALA:HA	5:F:299:TRP:HB3	1.90	0.53
2:C:239:PHE:CE1	2:C:246:ASP:HB3	2.44	0.53
3:N:147:VAL:HB	9:N:2267:HOH:O	2.07	0.53
3:D:1109:GLU:HA	9:D:2056:HOH:O	2.09	0.53
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.89	0.53
3:N:1301:LYS:HA	9:N:9307:HOH:O	2.08	0.53
3:D:71:LYS:HB2	9:D:9610:HOH:O	2.08	0.53
3:N:397:LYS:HG2	9:N:2124:HOH:O	2.07	0.53
5:P:81:VAL:HG13	9:P:4331:HOH:O	2.07	0.53
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.07	0.53
5:P:169:GLU:CD	5:P:169:GLU:H	2.11	0.53
2:C:571:LEU:HD13	2:C:670:GLN:OE1	2.08	0.53
3:D:1253:THR:HG23	3:D:1258:ARG:HH11	1.72	0.53
3:D:421:LEU:HG	9:D:2049:HOH:O	2.08	0.53
5:F:160:ASP:O	5:F:163:LEU:HB2	2.09	0.53
3:N:637:LEU:HD12	3:N:641:GLN:HG3	1.89	0.53
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.44	0.53
1:B:123:MET:C	1:B:125:PRO:HD3	2.28	0.53
1:A:44:LEU:HD22	9:A:9579:HOH:O	2.08	0.53
3:N:1459:LEU:HD12	3:N:1470:ARG:HH11	1.74	0.53
3:N:464:LEU:HA	9:N:2397:HOH:O	2.09	0.53
2:C:897:LEU:HD22	9:C:9860:HOH:O	2.08	0.53
2:C:36:PRO:HB3	9:C:9597:HOH:O	2.08	0.53
3:N:221:ALA:HB2	9:N:2049:HOH:O	2.08	0.53
3:D:470:LEU:HD11	3:D:509:PRO:HG3	1.90	0.53
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.89	0.53
5:F:403:LYS:HD3	9:F:9572:HOH:O	2.08	0.53
2:M:722:ILE:O	2:M:722:ILE:HG23	2.08	0.53
2:M:9:ILE:HG12	2:M:907:ASP:CG	2.28	0.53
3:N:429:SER:HA	9:N:2866:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:HIS:HB2	2:C:418:LEU:HD12	1.90	0.53
2:C:165:LEU:HA	2:C:166:PRO:O	2.08	0.53
3:D:584:ASN:H	3:D:602:SER:CB	2.21	0.53
1:L:97:VAL:HG23	9:L:7067:HOH:O	2.08	0.53
3:D:7:LYS:HE2	9:D:2085:HOH:O	2.09	0.53
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.91	0.53
2:M:12:VAL:HG12	2:M:534:VAL:HG13	1.91	0.53
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.89	0.53
2:C:721:ARG:HE	2:C:783:ARG:NH2	2.06	0.53
2:C:267:TYR:CE1	2:C:338:GLU:HG3	2.43	0.53
2:C:432:ARG:HG3	2:C:432:ARG:NH1	2.23	0.53
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.23	0.53
2:M:594:ALA:HB1	2:M:656:ALA:O	2.09	0.53
3:N:819:GLY:O	3:N:822:ALA:HB3	2.08	0.53
3:D:243:ALA:HB2	9:D:2875:HOH:O	2.09	0.53
3:N:854:ALA:HB2	9:N:9448:HOH:O	2.07	0.53
1:L:184:THR:HG22	1:L:192:LEU:O	2.07	0.53
3:N:1246:VAL:HG22	9:N:2507:HOH:O	2.08	0.53
3:D:961:LYS:HD2	9:D:9896:HOH:O	2.08	0.53
3:D:412:GLY:O	3:D:421:LEU:HB3	2.09	0.53
2:M:141:HIS:HE1	2:M:332:ARG:HD3	1.74	0.53
2:M:536:PRO:CG	2:M:906:PHE:HB2	2.39	0.53
1:A:213:GLN:O	1:A:217:ILE:HG13	2.08	0.53
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.91	0.53
2:M:1052:MET:SD	2:M:1056:LYS:HD3	2.48	0.53
2:C:1057:SER:OG	3:D:621:LYS:HG2	2.09	0.53
3:D:601:ARG:HH22	3:D:613:ARG:NE	2.06	0.53
2:C:759:THR:HG21	2:C:783:ARG:NH1	2.23	0.53
3:D:676:MET:CE	3:D:684:LYS:H	2.22	0.53
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.08	0.53
2:C:18:LEU:HD23	2:C:542:VAL:HG11	1.90	0.53
2:M:379:GLU:O	2:M:383:ARG:HB2	2.08	0.53
2:C:84:ARG:HA	9:C:9908:HOH:O	2.08	0.53
3:D:1173:LEU:HD22	9:D:9959:HOH:O	2.08	0.53
3:D:984:THR:HG23	3:D:986:ARG:H	1.73	0.53
3:D:1384:PRO:HB3	9:D:2732:HOH:O	2.09	0.53
3:D:489:ARG:HE	3:D:493:ARG:NH2	1.97	0.53
2:M:777:ILE:HG23	5:P:409:LYS:CB	2.31	0.53
2:C:874:LEU:HD11	3:D:784:ASP:HA	1.91	0.53
3:N:907:GLU:OE1	3:N:909:ASN:HB2	2.09	0.53
5:F:172:ARG:O	5:F:176:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:637:LEU:HD11	3:N:642:CYS:N	2.24	0.53
2:M:1056:LYS:HE2	9:M:9265:HOH:O	2.09	0.53
3:N:728:LEU:HD12	3:N:729:HIS:H	1.74	0.53
2:C:1102:LEU:HD11	3:D:9:ARG:HG2	1.90	0.53
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.39	0.53
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.28	0.53
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.08	0.53
1:B:206:THR:HB	1:B:209:GLU:OE2	2.09	0.53
3:D:1264:GLU:HG2	9:D:9600:HOH:O	2.07	0.53
5:P:76:SER:HB2	9:P:1916:HOH:O	2.08	0.53
4:E:15:SER:HA	9:E:9559:HOH:O	2.08	0.53
2:M:280:LYS:HG2	9:M:2041:HOH:O	2.09	0.53
3:D:138:LYS:HA	9:D:2798:HOH:O	2.09	0.53
2:C:929:ARG:HH11	2:C:929:ARG:HG3	1.73	0.53
4:O:27:ALA:O	4:O:31:LEU:HG	2.09	0.53
3:N:484:PRO:HB3	9:N:9533:HOH:O	2.09	0.53
1:B:23:PHE:HE1	1:B:208:LEU:HD13	1.74	0.53
3:D:865:THR:HG22	3:D:874:GLU:HG2	1.91	0.53
3:D:487:ALA:CB	3:D:488:ARG:HH21	2.22	0.53
5:F:132:ARG:HH21	5:F:184:ARG:NH1	2.06	0.53
3:D:1231:GLU:HG3	3:D:1232:PRO:N	2.23	0.53
1:B:175:ARG:HB2	1:B:200:TRP:HB3	1.91	0.53
2:M:225:SER:HB2	2:M:229:MET:HE2	1.91	0.53
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.24	0.53
5:P:234:LYS:HB2	9:P:4664:HOH:O	2.07	0.53
1:A:10:VAL:HG12	1:A:12:THR:HG23	1.90	0.53
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.90	0.53
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.90	0.53
3:N:1383:ASP:HB3	3:N:1416:ALA:H	1.74	0.53
2:C:26:TYR:CE2	2:C:30:LEU:HD21	2.43	0.53
3:N:1304:LYS:HD3	3:N:1304:LYS:H	1.74	0.53
5:F:420:ASP:HA	9:F:9593:HOH:O	2.08	0.53
3:D:564:GLU:HB3	9:D:9582:HOH:O	2.08	0.53
3:N:112:ILE:HG22	3:N:512:MET:SD	2.49	0.53
2:C:137:VAL:HG21	2:C:393:GLN:HE22	1.73	0.53
1:A:27:PRO:HB2	9:A:9811:HOH:O	2.08	0.53
2:C:976:ASP:HA	9:C:9567:HOH:O	2.09	0.53
4:O:41:GLU:HG2	9:O:1576:HOH:O	2.09	0.53
2:C:64:LEU:HD11	9:C:2120:HOH:O	2.08	0.53
2:C:876:VAL:H	2:C:877:PRO:HD2	1.74	0.53
2:M:142:ARG:HD3	9:M:2230:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:GLN:O	2:M:333:ILE:HA	2.08	0.53
1:L:87:VAL:HG23	9:L:1617:HOH:O	2.09	0.53
3:N:118:LEU:O	3:N:120:ALA:N	2.41	0.53
3:N:814:ALA:O	3:N:818:ARG:HG3	2.09	0.53
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.08	0.53
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.22	0.53
3:D:994:GLN:O	3:D:998:GLU:HG3	2.08	0.53
1:K:123:MET:C	1:K:125:PRO:HD3	2.29	0.53
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.24	0.53
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.39	0.53
1:L:182:GLU:HA	9:N:9281:HOH:O	2.09	0.53
2:M:713:ARG:O	2:M:720:GLU:HG3	2.09	0.53
2:M:150:PRO:HB2	9:M:9278:HOH:O	2.07	0.53
3:D:462:GLN:HG3	3:D:513:ILE:HD13	1.91	0.53
5:P:266:GLU:HG3	9:P:8061:HOH:O	2.08	0.53
1:B:176:ARG:HG3	1:B:200:TRP:CE3	2.44	0.53
2:M:473:ARG:HB3	9:M:9208:HOH:O	2.09	0.53
5:F:157:GLU:HA	9:F:2058:HOH:O	2.08	0.53
3:D:432:TYR:HA	3:D:448:GLU:O	2.08	0.53
2:C:455:LEU:HD13	2:C:459:ALA:HB3	1.91	0.53
1:K:96:THR:OG1	1:K:143:ARG:HD2	2.09	0.53
1:B:182:GLU:O	1:B:194:LYS:HB3	2.09	0.53
2:C:485:TYR:HD2	9:C:9588:HOH:O	1.90	0.53
3:N:608:SER:O	3:N:614:PHE:HB2	2.09	0.53
2:M:904:PRO:HG2	9:M:9888:HOH:O	2.08	0.53
2:C:193:LEU:HD13	2:C:193:LEU:O	2.09	0.53
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.09	0.53
2:C:423:ALA:HA	9:C:2245:HOH:O	2.09	0.53
3:N:187:LYS:HD3	9:N:9419:HOH:O	2.09	0.53
2:M:695:LEU:HD21	2:M:833:LEU:HB3	1.91	0.53
2:M:841:ASN:HD22	2:M:841:ASN:N	2.06	0.53
3:N:89:ARG:O	3:N:521:PRO:HG3	2.09	0.53
5:F:119:ILE:HD13	5:F:170:HIS:CG	2.44	0.53
3:D:1197:ARG:HD2	3:D:1396:GLU:CB	2.36	0.53
5:P:393:THR:CG2	5:P:394:ARG:H	2.22	0.53
2:M:290:LEU:HD13	2:M:290:LEU:H	1.73	0.53
2:C:751:PRO:HA	2:C:792:VAL:HB	1.89	0.53
3:D:804:LEU:HD12	3:D:831:GLY:HA3	1.90	0.53
1:L:136:GLY:HA3	9:L:1193:HOH:O	2.07	0.53
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.38	0.53
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.91	0.53
2:M:663:ASN:HB2	9:M:9366:HOH:O	2.08	0.53
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.44	0.53
3:N:1018:ASN:O	3:N:1022:VAL:HG23	2.09	0.53
3:D:1337:GLU:HA	9:D:9894:HOH:O	2.09	0.53
2:C:41:ASN:HD22	2:C:41:ASN:H	1.56	0.53
3:D:1383:ASP:HB3	3:D:1416:ALA:H	1.73	0.53
3:N:1320:GLU:H	3:N:1323:GLN:NE2	2.06	0.53
3:D:1495:ILE:HD12	3:D:1498:ALA:HB3	1.90	0.53
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	1.90	0.52
2:C:100:LEU:HD23	2:C:368:THR:HA	1.90	0.52
3:D:1020:LEU:HA	3:D:1023:MET:HE2	1.90	0.52
2:C:205:GLU:HB3	9:C:2115:HOH:O	2.09	0.52
5:F:315:VAL:HG12	5:F:316:SER:N	2.24	0.52
3:D:591:VAL:HG12	3:D:592:THR:O	2.09	0.52
3:D:98:PRO:O	3:D:458:ALA:HB3	2.08	0.52
2:M:186:VAL:HG23	2:M:187:ASN:H	1.73	0.52
1:B:178:ALA:C	1:B:198:ARG:HH21	2.12	0.52
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.91	0.52
2:C:114:PHE:HE2	5:F:283:GLY:HA3	1.73	0.52
3:D:1446:VAL:HG22	9:D:9970:HOH:O	2.09	0.52
2:M:637:LEU:HB2	9:M:9559:HOH:O	2.09	0.52
2:M:722:ILE:HG22	9:M:9639:HOH:O	2.09	0.52
1:K:227:ASN:HD22	1:K:227:ASN:H	1.56	0.52
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.09	0.52
1:B:2:LEU:HD12	1:B:3:ASP:N	2.24	0.52
1:B:5:LYS:HG3	9:B:9765:HOH:O	2.08	0.52
2:M:443:THR:HB	2:M:453:THR:HG22	1.91	0.52
5:F:376:ILE:HD13	9:F:2134:HOH:O	2.07	0.52
3:D:634:GLY:O	3:D:637:LEU:HB3	2.08	0.52
5:P:367:MET:HA	5:P:370:LYS:HD3	1.92	0.52
2:M:267:TYR:CE1	2:M:338:GLU:HG3	2.44	0.52
2:M:289:THR:O	2:M:291:ALA:N	2.42	0.52
2:M:602:GLU:HG2	2:M:603:VAL:N	2.24	0.52
3:D:819:GLY:O	3:D:822:ALA:HB3	2.09	0.52
1:L:165:ILE:HD12	1:L:165:ILE:O	2.09	0.52
1:L:212:ASN:O	1:L:215:VAL:HG22	2.09	0.52
2:C:805:ARG:HA	9:C:9907:HOH:O	2.10	0.52
1:A:73:GLU:HG3	1:A:130:ALA:HA	1.90	0.52
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.74	0.52
3:D:1173:LEU:HB3	9:D:9959:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.91	0.52
2:M:1009:SER:HB2	3:N:651:GLU:O	2.09	0.52
1:B:90:LEU:HB3	9:B:9609:HOH:O	2.09	0.52
2:M:774:LEU:O	2:M:777:ILE:HB	2.09	0.52
2:M:1101:THR:HB	3:N:5:VAL:CG1	2.39	0.52
2:M:165:LEU:HA	2:M:166:PRO:O	2.10	0.52
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.91	0.52
5:F:112:ALA:O	5:F:116:LEU:HG	2.10	0.52
4:O:48:MET:CB	4:O:54:LEU:HB2	2.39	0.52
4:O:57:ASP:H	4:O:58:PRO:HD3	1.75	0.52
3:D:1496:GLU:O	3:D:1500:LYS:HG3	2.09	0.52
5:F:357:ALA:O	5:F:361:LEU:HD23	2.09	0.52
3:N:1490:LYS:HE3	9:O:1697:HOH:O	2.10	0.52
2:C:752:GLY:N	2:C:792:VAL:HB	2.25	0.52
2:M:185:LYS:HD2	9:M:9853:HOH:O	2.08	0.52
1:K:36:LEU:O	1:K:39:PRO:HD2	2.09	0.52
3:N:792:ILE:HG23	3:N:793:THR:HG23	1.89	0.52
3:N:1014:ASN:O	3:N:1016:PRO:HD3	2.09	0.52
4:O:50:THR:HG22	9:O:1369:HOH:O	2.10	0.52
2:M:402:SER:HA	2:M:566:THR:HG23	1.92	0.52
3:D:439:LEU:HB3	9:D:2486:HOH:O	2.10	0.52
2:C:1001:VAL:HG13	9:C:9609:HOH:O	2.10	0.52
1:K:154:GLU:HA	9:M:9690:HOH:O	2.09	0.52
2:C:243:ARG:HD2	2:C:243:ARG:O	2.09	0.52
5:F:264:MET:O	5:F:268:ILE:HG13	2.09	0.52
5:F:323:ASP:O	5:F:325:LYS:HG3	2.10	0.52
3:N:1075:HIS:HA	9:N:9472:HOH:O	2.09	0.52
3:N:1378:TYR:HD1	3:N:1422:MET:SD	2.32	0.52
3:N:431:VAL:HG21	9:N:9483:HOH:O	2.08	0.52
2:M:237:ARG:HG3	9:M:9694:HOH:O	2.08	0.52
3:N:899:LEU:HD13	3:N:900:ILE:HG23	1.90	0.52
2:M:987:ILE:CG2	3:N:948:THR:HG21	2.39	0.52
3:D:972:LEU:HG	3:D:976:GLN:NE2	2.19	0.52
2:M:1014:SER:HA	5:P:334:PRO:HA	1.92	0.52
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.91	0.52
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.90	0.52
3:N:704:ARG:CD	3:N:705:ALA:H	2.21	0.52
3:N:1440:PHE:HB3	3:N:1442:ASN:ND2	2.24	0.52
1:B:45:LEU:HD21	1:B:177:VAL:HG23	1.90	0.52
3:D:690:ALA:O	3:D:694:VAL:HG23	2.10	0.52
2:M:17:PRO:HD3	9:M:9857:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1165:TYR:OH	3:D:1203:LYS:HD3	2.09	0.52
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.92	0.52
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.91	0.52
1:L:143:ARG:NE	1:L:158:ILE:HG21	2.24	0.52
4:E:83:ASP:HA	9:E:9560:HOH:O	2.09	0.52
2:C:294:GLU:HB2	9:C:2038:HOH:O	2.09	0.52
5:P:392:VAL:HG13	9:P:6344:HOH:O	2.09	0.52
2:C:965:GLU:HA	9:C:2351:HOH:O	2.09	0.52
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.08	0.52
3:D:228:ALA:HA	9:D:9867:HOH:O	2.10	0.52
3:N:518:PRO:HB3	9:N:9475:HOH:O	2.09	0.52
9:M:9280:HOH:O	3:N:952:ASP:HB3	2.09	0.52
3:D:169:TYR:HA	3:D:392:SER:HA	1.91	0.52
3:D:970:LYS:HD2	9:D:2768:HOH:O	2.09	0.52
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.90	0.52
2:M:651:LYS:HB3	9:M:9725:HOH:O	2.09	0.52
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	2.08	0.52
3:D:8:VAL:HG12	3:D:1434:TRP:HH2	1.74	0.52
2:C:136:ILE:HD13	2:C:392:SER:HB2	1.92	0.52
2:C:266:ARG:HB2	2:C:288:ARG:HE	1.75	0.52
3:D:817:GLU:O	3:D:821:VAL:HG23	2.09	0.52
3:N:828:LYS:HE3	9:N:9267:HOH:O	2.09	0.52
3:N:1277:ILE:HD11	9:N:2604:HOH:O	2.08	0.52
2:C:682:TYR:HA	3:D:635:PRO:HG2	1.91	0.52
2:C:435:TYR:O	2:C:437:ARG:HG3	2.09	0.52
5:P:295:MET:HB3	5:P:299:TRP:CD1	2.44	0.52
5:P:123:ASP:HB3	5:P:125:ASP:OD1	2.09	0.52
1:L:184:THR:O	1:L:192:LEU:HB2	2.09	0.52
5:F:96:LEU:HB2	9:F:9854:HOH:O	2.09	0.52
3:N:1284:GLU:HB3	9:N:2710:HOH:O	2.08	0.52
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.90	0.52
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.75	0.52
2:M:599:GLU:HG2	9:M:9329:HOH:O	2.09	0.52
1:K:42:ARG:NH1	9:K:1228:HOH:O	2.41	0.52
3:D:498:VAL:HG13	9:D:2123:HOH:O	2.10	0.52
4:O:40:LEU:HD12	4:O:40:LEU:O	2.09	0.52
5:P:364:ARG:HB3	5:P:365:GLU:OE1	2.10	0.52
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.10	0.52
2:C:267:TYR:HA	9:C:9947:HOH:O	2.08	0.52
2:M:725:ASP:HB3	2:M:783:ARG:NH1	2.25	0.52
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.25	0.52
3:D:1410:GLU:HA	9:D:9597:HOH:O	2.08	0.52
3:N:583:ASP:HA	3:N:602:SER:OG	2.09	0.52
5:F:376:ILE:HD12	9:F:2054:HOH:O	2.10	0.52
3:D:643:GLY:HA3	3:D:727:GLN:HG3	1.92	0.52
4:O:51:LEU:C	4:O:53:GLY:H	2.12	0.52
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.90	0.52
2:C:594:ALA:HB1	2:C:656:ALA:O	2.09	0.52
3:D:480:GLU:O	3:D:484:PRO:HD2	2.10	0.52
3:N:493:ARG:O	3:N:497:GLU:HG3	2.10	0.52
2:M:1054:THR:HG23	2:M:1059:ASP:CB	2.39	0.52
8:N:9101:G4P:H4'	9:N:9248:HOH:O	2.10	0.52
2:C:838:LYS:HD2	2:C:846:LYS:HZ1	1.75	0.52
2:C:1008:ARG:HD2	2:C:1028:GLY:C	2.30	0.52
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.74	0.52
2:C:1015:LEU:HD12	5:F:333:ILE:HG21	1.92	0.52
2:M:589:ARG:HD3	2:M:596:TYR:CE2	2.45	0.52
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.92	0.52
1:L:125:PRO:HD2	9:L:2226:HOH:O	2.09	0.52
9:D:9641:HOH:O	5:F:375:LEU:HD11	2.08	0.52
3:N:1465:ASN:HD21	3:N:1470:ARG:CZ	2.23	0.52
1:A:125:PRO:HB2	9:A:9597:HOH:O	2.10	0.52
3:N:1433:SER:HB2	3:N:1457:ASP:CG	2.30	0.52
3:N:601:ARG:HB2	5:P:318:GLU:CD	2.30	0.52
1:B:20:TYR:HE2	1:B:198:ARG:HB3	1.74	0.52
2:M:383:ARG:HG2	9:M:9403:HOH:O	2.09	0.52
1:B:184:THR:O	1:B:192:LEU:HB2	2.10	0.52
3:D:1478:SER:HA	9:D:9950:HOH:O	2.10	0.52
5:P:203:THR:HG22	9:P:4204:HOH:O	2.09	0.52
2:C:597:ALA:HA	9:C:9658:HOH:O	2.10	0.52
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.91	0.52
3:D:191:LEU:CB	3:D:195:VAL:HG21	2.37	0.52
3:N:119:SER:HB2	3:N:123:LEU:CB	2.35	0.52
2:M:129:ILE:HG22	2:M:130:ASN:H	1.73	0.52
3:N:524:LEU:C	3:N:526:PRO:HD3	2.30	0.52
2:C:534:VAL:N	2:C:538:GLN:HE22	2.08	0.52
1:A:50:GLY:CA	1:A:173:PRO:HG3	2.39	0.52
2:M:949:LYS:NZ	3:N:796:ARG:HH22	2.08	0.52
1:A:176:ARG:HD2	9:A:9580:HOH:O	2.10	0.52
2:M:727:PRO:HG3	2:M:783:ARG:NH1	2.25	0.52
3:D:152:LEU:HD23	3:D:152:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:875:THR:HG21	3:N:902:LEU:HD12	1.92	0.52
3:D:431:VAL:HG11	9:D:9858:HOH:O	2.10	0.52
2:M:771:GLU:HB2	9:M:9677:HOH:O	2.09	0.52
5:P:395:GLU:O	5:P:399:GLN:HB2	2.09	0.52
3:D:507:ASN:HA	9:D:9571:HOH:O	2.08	0.52
3:N:657:LEU:HD13	3:N:691:LEU:HA	1.91	0.52
5:F:259:ARG:HG2	5:F:259:ARG:HH11	1.74	0.52
2:C:216:GLU:HG2	2:C:217:LEU:HD23	1.91	0.52
1:A:14:ARG:HG2	9:A:9563:HOH:O	2.09	0.52
3:D:1104:GLU:OE2	3:D:1432:LYS:HE2	2.10	0.52
3:N:215:TYR:O	3:N:389:GLU:HB3	2.10	0.52
2:M:690:ILE:HG12	2:M:849:VAL:HG13	1.91	0.52
2:C:841:ASN:C	2:C:841:ASN:HD22	2.12	0.52
3:N:141:ILE:HB	9:N:9513:HOH:O	2.09	0.52
5:F:270:LYS:HE2	9:F:2083:HOH:O	2.09	0.52
3:N:909:ASN:HA	3:N:912:LYS:HZ2	1.74	0.52
9:M:9265:HOH:O	3:N:751:LEU:HG	2.10	0.52
5:F:135:ILE:CD1	5:F:178:ARG:HD2	2.39	0.52
1:A:153:ALA:HB3	9:A:9823:HOH:O	2.09	0.52
5:P:270:LYS:HD3	9:P:5561:HOH:O	2.09	0.52
3:N:1403:LEU:HD23	9:N:9392:HOH:O	2.10	0.52
1:L:12:THR:HB	9:L:8156:HOH:O	2.08	0.52
2:C:242:LEU:HA	9:C:9763:HOH:O	2.08	0.52
2:C:620:LEU:HA	9:C:9918:HOH:O	2.08	0.52
1:L:42:ARG:HH11	1:L:42:ARG:HG2	1.74	0.52
2:C:224:GLU:OE1	2:C:226:VAL:HB	2.09	0.52
3:D:1132:LEU:HB2	9:D:2139:HOH:O	2.10	0.52
3:N:414:ARG:HG2	9:N:9972:HOH:O	2.10	0.52
3:N:459:GLU:O	3:N:463:GLN:HG2	2.09	0.52
2:M:206:THR:O	2:M:210:GLU:HB2	2.09	0.52
9:M:9336:HOH:O	5:P:342:VAL:HA	2.09	0.52
2:M:786:LYS:HA	9:M:9432:HOH:O	2.09	0.52
1:A:61:VAL:HA	9:A:9599:HOH:O	2.08	0.52
3:N:1258:ARG:NH2	3:N:1262:LEU:HD11	2.25	0.52
3:D:804:LEU:HD12	3:D:804:LEU:O	2.10	0.52
1:L:194:LYS:HG2	9:L:1718:HOH:O	2.10	0.52
2:C:606:VAL:HG21	2:C:645:VAL:HG22	1.91	0.52
5:F:185:GLN:HA	5:F:188:ILE:HD12	1.92	0.52
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.92	0.52
5:P:214:GLN:O	5:P:217:ASN:HB2	2.10	0.52
2:M:604:ALA:HB3	2:M:612:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:866:PRO:HD2	9:C:2231:HOH:O	2.09	0.52
2:C:420:ARG:HD3	9:C:9964:HOH:O	2.09	0.52
2:M:55:GLU:HG3	9:M:2409:HOH:O	2.09	0.52
1:A:51:THR:HG23	9:A:9681:HOH:O	2.08	0.52
4:O:33:HIS:CG	4:O:89:MET:HG2	2.45	0.52
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.92	0.52
2:C:791:ARG:HB2	9:C:2241:HOH:O	2.09	0.52
3:D:422:ALA:H	3:D:427:VAL:HG11	1.75	0.51
3:N:65:ARG:CG	5:P:375:LEU:HD12	2.40	0.51
3:N:692:GLU:CG	3:N:720:LEU:HD12	2.40	0.51
5:P:340:SER:O	5:P:342:VAL:N	2.43	0.51
2:C:166:PRO:HD2	9:C:9681:HOH:O	2.09	0.51
3:D:623:VAL:HG12	3:D:625:TYR:H	1.75	0.51
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.92	0.51
1:L:175:ARG:HB2	1:L:200:TRP:HB3	1.91	0.51
2:M:284:ARG:HD3	9:M:2023:HOH:O	2.10	0.51
3:D:1127:GLU:HB2	9:D:9997:HOH:O	2.09	0.51
1:A:177:VAL:O	2:C:864:GLY:HA2	2.09	0.51
2:C:250:ARG:HG2	9:C:9691:HOH:O	2.10	0.51
5:P:158:GLU:HA	5:P:161:GLN:NE2	2.25	0.51
2:C:503:LEU:HD23	9:C:2771:HOH:O	2.09	0.51
1:K:189:ARG:HD3	9:K:2051:HOH:O	2.10	0.51
2:M:755:LEU:HD11	2:M:792:VAL:HA	1.92	0.51
3:N:971:LEU:O	3:N:975:GLU:HG2	2.09	0.51
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.91	0.51
1:B:160:ASP:HB2	9:B:9744:HOH:O	2.10	0.51
2:C:1096:ALA:O	3:D:13:ALA:HB2	2.10	0.51
3:N:197:SER:HB2	3:N:205:TYR:HE1	1.72	0.51
3:N:98:PRO:CG	3:N:462:GLN:HE22	2.17	0.51
3:N:1137:ARG:CD	3:N:1137:ARG:H	2.13	0.51
2:C:166:PRO:HG2	9:C:9694:HOH:O	2.09	0.51
3:N:853:VAL:HG13	3:N:858:VAL:O	2.09	0.51
2:C:1017:THR:HG23	9:C:9664:HOH:O	2.09	0.51
3:D:609:GLY:CA	3:D:613:ARG:HB3	2.40	0.51
2:C:773:LEU:HD23	2:C:774:LEU:N	2.24	0.51
3:N:1038:LEU:HA	3:N:1061:PHE:HB2	1.92	0.51
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.31	0.51
4:E:51:LEU:HG	4:E:53:GLY:N	2.26	0.51
9:N:9482:HOH:O	5:P:132:ARG:HD3	2.10	0.51
2:M:756:VAL:O	2:M:789:SER:HB3	2.09	0.51
1:B:126:ASP:HA	9:B:9726:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:475:LYS:O	3:N:478:LEU:HB2	2.10	0.51
2:C:99:GLN:HA	9:C:2465:HOH:O	2.08	0.51
5:F:110:MET:O	5:F:114:LYS:HG3	2.10	0.51
1:K:29:GLU:HB2	9:K:2006:HOH:O	2.10	0.51
3:D:56:TYR:O	3:D:80:VAL:HG11	2.10	0.51
1:B:101:LEU:HA	9:B:9586:HOH:O	2.09	0.51
3:N:732:VAL:HG11	3:N:765:SER:OG	2.10	0.51
2:M:735:ARG:HD2	9:M:2232:HOH:O	2.10	0.51
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.09	0.51
2:M:164:PRO:HB3	9:M:9286:HOH:O	2.09	0.51
3:N:984:THR:CG2	3:N:987:GLU:H	2.23	0.51
2:M:230:ARG:NH1	9:M:9242:HOH:O	2.43	0.51
5:F:393:THR:HA	9:F:9726:HOH:O	2.09	0.51
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.92	0.51
2:M:597:ALA:HB1	9:M:9609:HOH:O	2.09	0.51
2:C:288:ARG:HG3	2:C:289:THR:N	2.26	0.51
2:M:312:ALA:HB1	2:M:318:PRO:CG	2.39	0.51
3:N:679:ARG:HG2	3:N:681:ARG:HD3	1.92	0.51
2:M:444:PRO:HD2	2:M:452:ILE:HG13	1.92	0.51
5:F:144:ILE:HG23	9:F:9661:HOH:O	2.11	0.51
3:D:881:LEU:HD11	3:D:884:ARG:NH2	2.25	0.51
2:C:252:LYS:HE3	9:C:2326:HOH:O	2.10	0.51
1:K:155:LYS:HE3	9:K:2316:HOH:O	2.09	0.51
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.75	0.51
2:M:798:GLY:H	2:M:827:VAL:CG1	2.23	0.51
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.93	0.51
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.11	0.51
3:D:984:THR:CG2	3:D:987:GLU:H	2.24	0.51
3:D:699:VAL:CG1	3:D:717:GLN:HG2	2.41	0.51
2:M:140:ILE:HG22	2:M:331:ARG:HB3	1.93	0.51
9:C:9793:HOH:O	3:D:90:MET:HB2	2.10	0.51
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.40	0.51
1:L:91:ASN:O	1:L:94:LEU:HD12	2.10	0.51
2:C:1101:THR:HG22	3:D:8:VAL:HG22	1.91	0.51
3:N:768:ASN:HB3	9:N:9759:HOH:O	2.11	0.51
2:C:1069:ALA:HA	2:C:1074:GLU:OE1	2.10	0.51
5:F:140:ARG:HG3	5:F:141:VAL:N	2.26	0.51
3:N:550:ARG:NH1	3:N:550:ARG:HG3	2.23	0.51
3:N:602:SER:HB3	9:N:9292:HOH:O	2.11	0.51
3:N:1412:LYS:O	3:N:1412:LYS:HG3	2.10	0.51
5:P:139:ALA:HB1	5:P:152:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:90:GLU:HG3	9:E:9578:HOH:O	2.10	0.51
1:B:194:LYS:HG2	9:B:9628:HOH:O	2.11	0.51
5:P:392:VAL:HG12	5:P:396:ARG:HB2	1.92	0.51
3:D:1411:GLY:O	3:D:1413:THR:HG23	2.10	0.51
3:D:889:ALA:O	3:D:929:ARG:HD2	2.11	0.51
2:M:120:LEU:O	2:M:127:PHE:HD1	1.94	0.51
3:N:1244:GLY:HA3	9:N:9415:HOH:O	2.11	0.51
3:D:1309:ALA:HA	9:D:9716:HOH:O	2.11	0.51
1:K:42:ARG:NH1	9:K:4396:HOH:O	2.43	0.51
3:D:699:VAL:N	3:D:756:GLN:HE22	2.09	0.51
3:D:486:ARG:HA	3:D:486:ARG:HE	1.76	0.51
5:P:366:ALA:O	5:P:370:LYS:HB3	2.10	0.51
2:M:260:LEU:HA	2:M:291:ALA:CB	2.39	0.51
2:C:218:VAL:O	2:C:221:LEU:HB3	2.11	0.51
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.25	0.51
5:F:273:ARG:HA	5:F:276:ARG:NH1	2.23	0.51
2:C:1014:SER:CB	5:F:331:ASP:HA	2.40	0.51
3:D:1497:GLU:O	3:D:1501:GLU:HG3	2.10	0.51
3:D:609:GLY:HA2	3:D:613:ARG:HB3	1.92	0.51
9:C:9824:HOH:O	5:F:373:LYS:HB3	2.09	0.51
2:M:824:ARG:HD3	9:M:9630:HOH:O	2.11	0.51
5:F:314:PRO:HB2	9:F:9559:HOH:O	2.09	0.51
1:K:123:MET:HB3	9:K:1711:HOH:O	2.09	0.51
2:C:54:ILE:HG23	2:C:54:ILE:O	2.10	0.51
3:D:28:LYS:HD2	3:D:41:ARG:CD	2.41	0.51
2:M:697:ARG:HG3	9:M:9636:HOH:O	2.09	0.51
2:M:524:VAL:HG22	2:M:525:SER:N	2.26	0.51
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.46	0.51
9:M:2120:HOH:O	4:O:32:ARG:HA	2.09	0.51
2:M:279:GLU:HG3	2:M:280:LYS:N	2.26	0.51
3:N:101:HIS:HD2	3:N:582:LEU:HD13	1.75	0.51
3:D:1013:GLU:HG3	9:D:9868:HOH:O	2.10	0.51
3:D:402:PRO:HB3	9:D:9656:HOH:O	2.09	0.51
3:N:186:VAL:HG11	3:N:213:VAL:HB	1.93	0.51
5:F:126:LEU:O	5:F:130:VAL:HG23	2.11	0.51
5:P:404:ALA:HB2	9:P:7921:HOH:O	2.09	0.51
1:L:206:THR:CG2	1:L:209:GLU:H	2.23	0.51
2:C:857:ASP:HB2	2:C:978:ARG:CG	2.39	0.51
2:M:651:LYS:HE3	9:M:9350:HOH:O	2.10	0.51
2:C:182:VAL:HG12	9:C:9945:HOH:O	2.11	0.51
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:ILE:HG22	9:C:2143:HOH:O	2.11	0.51
1:A:146:ARG:HG3	9:A:9567:HOH:O	2.11	0.51
2:C:861:LEU:HD23	2:C:863:ASP:N	2.26	0.51
1:A:45:LEU:HD21	9:A:9583:HOH:O	2.11	0.51
1:B:129:ILE:HG23	9:B:9809:HOH:O	2.10	0.51
2:C:476:GLY:C	2:C:478:VAL:H	2.14	0.51
2:M:455:LEU:HD13	2:M:456:ALA:O	2.10	0.51
3:N:893:GLU:HA	9:N:9628:HOH:O	2.10	0.51
3:D:1264:GLU:O	3:D:1266:ARG:HG3	2.10	0.51
2:M:674:VAL:HG23	2:M:869:VAL:O	2.11	0.51
3:N:1368:ILE:O	3:N:1372:VAL:HG23	2.10	0.51
2:M:1045:ALA:HA	3:N:758:GLU:OE1	2.11	0.51
1:B:6:LEU:C	1:B:8:ALA:H	2.14	0.51
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.92	0.51
2:M:1108:PRO:HD2	9:M:2092:HOH:O	2.10	0.51
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.93	0.51
3:D:493:ARG:HD2	3:D:1390:LEU:HD21	1.92	0.51
3:N:67:ARG:CD	5:P:375:LEU:HD11	2.36	0.51
2:C:1088:LEU:O	2:C:1091:GLU:HB2	2.11	0.51
3:D:171:LEU:HG	9:D:3222:HOH:O	2.11	0.51
3:D:770:LEU:HA	9:D:9581:HOH:O	2.11	0.51
2:M:603:VAL:O	2:M:646:GLY:HA2	2.11	0.51
3:D:809:PRO:O	3:D:812:ALA:HB3	2.11	0.51
1:B:51:THR:HA	1:B:171:PHE:HD1	1.76	0.51
3:D:162:ARG:HG3	3:D:163:TYR:N	2.26	0.51
2:C:276:LYS:HD3	9:C:2144:HOH:O	2.10	0.51
3:N:474:GLU:O	3:N:478:LEU:HG	2.10	0.51
3:N:1044:LEU:HD21	3:N:1056:PRO:HG3	1.92	0.51
3:D:581:LEU:H	3:D:581:LEU:HD23	1.75	0.51
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.46	0.51
3:D:853:VAL:HG13	3:D:858:VAL:O	2.11	0.51
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.10	0.51
3:N:1087:ARG:NE	3:N:1238:MET:HB2	2.26	0.51
2:M:331:ARG:HG2	9:M:9957:HOH:O	2.10	0.51
3:N:800:LYS:HG2	3:N:829:VAL:CG1	2.37	0.51
2:M:195:LEU:O	2:M:199:VAL:HG23	2.11	0.51
2:M:205:GLU:HA	2:M:209:ARG:NH2	2.25	0.51
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.38	0.51
1:L:79:ILE:HA	1:L:82:LEU:HD12	1.93	0.51
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.92	0.51
3:N:701:LEU:O	3:N:747:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:111:ALA:HB3	1:K:124:ASN:O	2.10	0.51
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.93	0.51
3:N:1432:LYS:HG3	3:N:1433:SER:H	1.76	0.51
5:F:194:LEU:HB2	9:F:9560:HOH:O	2.09	0.51
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.92	0.51
3:D:783:ARG:NH1	3:D:1029:ARG:HD3	2.26	0.51
2:C:583:LEU:O	2:C:587:VAL:HG23	2.10	0.51
3:D:174:GLY:HA3	9:D:9734:HOH:O	2.09	0.51
3:N:179:VAL:HG13	9:N:2353:HOH:O	2.10	0.51
2:M:911:GLU:O	2:M:915:LYS:HG2	2.10	0.51
3:N:32:ILE:O	5:P:258:ILE:HG23	2.11	0.51
2:M:140:ILE:HA	2:M:332:ARG:O	2.11	0.51
2:M:266:ARG:H	2:M:288:ARG:NH1	2.09	0.51
2:M:431:HIS:CD2	2:M:433:THR:H	2.29	0.51
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.37	0.51
5:F:305:GLU:HG2	5:F:309:LYS:HE3	1.93	0.51
2:C:694:LEU:CD1	2:C:868:ASP:HB3	2.38	0.51
2:C:1021:LEU:HD12	3:D:622:ARG:HH12	1.75	0.51
1:K:119:ASP:HB3	9:K:1333:HOH:O	2.10	0.51
3:D:8:VAL:HG12	3:D:1434:TRP:CH2	2.45	0.51
4:O:87:LYS:HB2	9:O:2278:HOH:O	2.11	0.51
1:K:166:PRO:HA	9:K:2046:HOH:O	2.10	0.51
3:D:141:ILE:HD13	3:D:450:TYR:N	2.26	0.51
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.93	0.51
5:P:350:LEU:HD12	5:P:422:LEU:HD13	1.92	0.51
5:P:260:ILE:HG12	5:P:264:MET:HB2	1.92	0.51
3:D:1196:THR:HA	9:D:9591:HOH:O	2.10	0.51
1:A:145:ASP:HB3	9:A:9570:HOH:O	2.10	0.51
2:M:901:TYR:CE2	2:M:917:LEU:HD13	2.46	0.51
3:D:1212:ALA:HB1	9:D:2669:HOH:O	2.10	0.51
3:D:1388:ARG:HB2	9:D:2873:HOH:O	2.11	0.51
9:M:9230:HOH:O	5:P:405:LEU:HG	2.11	0.51
3:D:770:LEU:HD21	3:D:919:PHE:CE1	2.46	0.51
2:M:368:THR:HG22	9:M:9372:HOH:O	2.11	0.51
2:C:339:LEU:HD13	2:C:391:LEU:HD21	1.93	0.51
4:O:72:ARG:HG3	9:O:1901:HOH:O	2.11	0.51
2:C:723:THR:C	2:C:725:ASP:H	2.14	0.51
2:M:694:LEU:HD23	2:M:697:ARG:HH21	1.75	0.51
2:C:121:MET:HA	2:C:127:PHE:CD2	2.45	0.51
2:M:70:GLU:OE1	2:M:97:ARG:HD3	2.10	0.51
1:A:23:PHE:O	1:A:196:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1264:GLU:HG2	9:D:2050:HOH:O	2.11	0.51
2:C:70:GLU:HB3	9:C:9688:HOH:O	2.11	0.51
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.76	0.51
3:D:80:VAL:HA	9:D:2231:HOH:O	2.11	0.51
1:K:175:ARG:HD3	9:K:2112:HOH:O	2.10	0.51
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.11	0.51
1:B:227:ASN:HB2	9:B:9778:HOH:O	2.11	0.51
1:L:187:GLY:HA2	9:N:2058:HOH:O	2.10	0.51
3:N:9:ARG:HH11	3:N:9:ARG:HG2	1.74	0.50
3:N:1481:VAL:CG1	4:O:18:ARG:HA	2.36	0.50
5:F:304:VAL:HG12	5:F:308:LEU:HD11	1.91	0.50
2:C:118:ILE:H	2:C:118:ILE:CD1	2.23	0.50
3:D:777:PRO:O	3:D:912:LYS:HE3	2.11	0.50
2:C:332:ARG:HG2	2:C:465:GLY:HA3	1.92	0.50
3:D:1376:MET:SD	3:D:1421:LEU:HD13	2.51	0.50
3:N:645:PRO:HA	3:N:721:VAL:O	2.11	0.50
2:M:73:LEU:HG	9:M:9263:HOH:O	2.11	0.50
3:N:1312:LEU:HD12	3:N:1326:THR:O	2.12	0.50
3:N:813:LEU:HD21	9:N:9724:HOH:O	2.09	0.50
2:C:283:ILE:HB	2:C:284:ARG:HD2	1.92	0.50
2:C:470:PRO:HG2	9:C:9634:HOH:O	2.11	0.50
3:D:812:ALA:O	3:D:816:HIS:HB2	2.11	0.50
4:O:39:VAL:HB	4:O:72:ARG:HD3	1.93	0.50
1:B:162:ILE:HD12	9:B:9818:HOH:O	2.11	0.50
2:C:63:GLY:HA3	2:C:103:LYS:CG	2.41	0.50
3:N:601:ARG:NE	3:N:613:ARG:HH21	2.09	0.50
1:K:227:ASN:N	1:K:227:ASN:HD22	2.08	0.50
3:D:1313:VAL:HA	9:D:9855:HOH:O	2.11	0.50
4:E:70:THR:HA	9:E:9683:HOH:O	2.11	0.50
2:M:928:LYS:HG3	2:M:932:GLU:HG3	1.92	0.50
3:D:626:SER:HB3	3:D:748:HIS:ND1	2.27	0.50
2:M:27:ARG:HG3	2:M:27:ARG:HH11	1.76	0.50
5:P:128:ARG:HB2	5:P:128:ARG:NH1	2.26	0.50
3:N:1307:LYS:HG3	9:N:9927:HOH:O	2.11	0.50
2:C:61:LYS:HG3	9:C:2460:HOH:O	2.10	0.50
2:M:520:GLU:HG3	9:M:9551:HOH:O	2.11	0.50
3:N:156:GLU:HB3	9:N:9891:HOH:O	2.11	0.50
3:D:953:ASP:HA	9:D:9611:HOH:O	2.10	0.50
5:F:271:LEU:HD22	5:F:291:ILE:HD11	1.93	0.50
2:M:310:LEU:O	2:M:314:THR:HG23	2.11	0.50
3:D:868:TYR:HB2	3:D:873:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:140:ARG:HA	9:P:7056:HOH:O	2.10	0.50
2:M:182:VAL:HG23	9:M:9649:HOH:O	2.10	0.50
2:C:1100:GLN:HB3	9:D:9712:HOH:O	2.09	0.50
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.93	0.50
3:D:1346:ARG:HA	3:D:1346:ARG:NE	2.26	0.50
1:L:112:ARG:HG3	9:L:6646:HOH:O	2.11	0.50
4:E:51:LEU:HD13	9:E:9663:HOH:O	2.10	0.50
1:K:23:PHE:O	1:K:196:THR:HA	2.11	0.50
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.14	0.50
1:L:26:GLU:CB	1:L:194:LYS:HG3	2.41	0.50
1:A:18:ARG:HH22	1:A:88:ARG:NH2	2.09	0.50
1:A:18:ARG:NH2	1:A:88:ARG:HH21	2.07	0.50
2:C:478:VAL:HA	2:C:506:ASN:O	2.11	0.50
5:F:93:LEU:HD21	5:F:102:LEU:HD11	1.92	0.50
3:D:596:SER:C	3:D:598:ARG:H	2.14	0.50
3:N:1493:LYS:HD2	9:N:2553:HOH:O	2.11	0.50
3:D:827:ILE:O	3:D:837:GLY:HA3	2.11	0.50
3:D:550:ARG:HG3	3:D:550:ARG:HH11	1.76	0.50
3:N:1063:GLU:HB3	9:N:2394:HOH:O	2.11	0.50
1:B:12:THR:OG1	1:B:24:VAL:HB	2.11	0.50
1:A:198:ARG:HH22	2:C:932:GLU:CD	2.13	0.50
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.94	0.50
2:C:545:ASN:O	2:C:905:ILE:HD11	2.11	0.50
1:B:62:LEU:H	1:B:62:LEU:HD12	1.75	0.50
2:M:945:ARG:O	2:M:948:GLU:HG3	2.11	0.50
3:N:1128:VAL:HA	9:N:2136:HOH:O	2.10	0.50
1:A:152:PRO:HB3	9:C:9586:HOH:O	2.10	0.50
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.47	0.50
2:M:969:GLN:HB3	9:M:9280:HOH:O	2.10	0.50
2:M:952:LEU:CD1	2:M:969:GLN:HE22	2.19	0.50
2:C:157:ARG:HH11	2:C:157:ARG:HG3	1.76	0.50
2:M:1083:GLU:N	9:M:9233:HOH:O	2.43	0.50
2:M:1087:VAL:HG12	2:M:1091:GLU:OE2	2.11	0.50
2:M:195:LEU:HA	9:M:9289:HOH:O	2.12	0.50
2:M:568:ALA:CB	2:M:668:LEU:HB3	2.40	0.50
1:A:143:ARG:HD3	1:A:158:ILE:HG21	1.93	0.50
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.41	0.50
3:D:838:ARG:CG	3:D:865:THR:HG23	2.41	0.50
2:C:756:VAL:HG21	2:C:823:VAL:CG1	2.41	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.11	0.50
5:F:94:LEU:HB2	5:F:98:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:SG	3:D:59:ALA:N	2.83	0.50
1:A:186:LEU:HA	9:A:9786:HOH:O	2.11	0.50
1:L:2:LEU:HA	1:L:6:LEU:HD22	1.92	0.50
5:P:167:PRO:HB2	5:P:169:GLU:OE1	2.11	0.50
5:P:396:ARG:HA	5:P:399:GLN:HE21	1.76	0.50
2:C:965:GLU:HG3	9:C:2351:HOH:O	2.11	0.50
3:D:416:ALA:H	3:D:417:PRO:CD	2.25	0.50
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.93	0.50
2:C:799:ILE:O	2:C:801:VAL:HG13	2.11	0.50
3:N:1476:THR:HG23	4:O:21:VAL:CG2	2.41	0.50
3:D:1362:LYS:HE3	9:D:9887:HOH:O	2.10	0.50
2:M:41:ASN:HD22	2:M:41:ASN:H	1.58	0.50
1:K:171:PHE:O	1:K:172:SER:C	2.50	0.50
2:C:55:GLU:HG2	9:C:2166:HOH:O	2.11	0.50
3:D:1284:GLU:HB3	9:D:9836:HOH:O	2.11	0.50
2:C:1058:ASP:OD1	2:C:1084:SER:N	2.43	0.50
3:D:475:LYS:HD3	3:D:478:LEU:CD1	2.40	0.50
2:M:31:GLN:HB2	9:M:9742:HOH:O	2.10	0.50
2:M:431:HIS:HD2	2:M:433:THR:H	1.60	0.50
2:M:149:THR:HA	9:M:9241:HOH:O	2.11	0.50
2:M:516:ARG:CZ	3:N:1068:LEU:HD22	2.41	0.50
2:C:259:GLY:HA2	2:C:290:LEU:O	2.10	0.50
2:M:15:LEU:HD22	9:M:9656:HOH:O	2.12	0.50
9:M:2444:HOH:O	3:N:744:GLN:HG3	2.12	0.50
3:N:1127:GLU:HA	9:N:2957:HOH:O	2.10	0.50
2:C:725:ASP:O	2:C:727:PRO:HD3	2.11	0.50
3:D:1128:VAL:HB	3:D:1131:SER:OG	2.12	0.50
5:P:93:LEU:HD12	5:P:191:ASN:HD21	1.76	0.50
2:M:744:ARG:HA	9:M:9460:HOH:O	2.10	0.50
2:C:345:ARG:HD3	9:C:9778:HOH:O	2.10	0.50
3:N:596:SER:C	3:N:598:ARG:H	2.15	0.50
2:C:53:PRO:HG3	9:C:9996:HOH:O	2.10	0.50
2:C:745:ILE:HG12	9:C:9595:HOH:O	2.11	0.50
2:M:678:PRO:O	3:N:943:THR:HG23	2.12	0.50
2:C:108:ILE:HB	9:C:9838:HOH:O	2.12	0.50
1:L:180:GLN:HG2	9:L:1240:HOH:O	2.10	0.50
5:P:367:MET:HB3	9:P:3256:HOH:O	2.10	0.50
3:N:13:ALA:HB1	3:N:18:ILE:HD11	1.94	0.50
3:D:22:SER:HA	3:D:90:MET:O	2.12	0.50
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.42	0.50
3:D:132:TYR:CD1	3:D:132:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:17:LYS:HG3	9:N:9504:HOH:O	2.10	0.50
2:M:516:ARG:HB2	9:M:9549:HOH:O	2.11	0.50
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.45	0.50
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.37	0.50
3:N:1121:PRO:HD3	3:N:1346:ARG:HH22	1.76	0.50
1:B:111:ALA:HB3	1:B:124:ASN:O	2.11	0.50
3:N:165:LYS:HE2	9:N:9671:HOH:O	2.12	0.50
5:P:94:LEU:HD12	5:P:97:GLU:HB2	1.93	0.50
2:C:479:VAL:HG22	2:C:506:ASN:O	2.12	0.50
5:P:260:ILE:HD11	5:P:264:MET:HB3	1.94	0.50
2:C:426:ASP:HA	2:C:429:ASP:OD2	2.12	0.50
1:A:46:SER:HA	9:A:9582:HOH:O	2.11	0.50
3:N:102:ILE:HD13	3:N:586:ARG:HB2	1.94	0.50
2:M:28:ARG:HG2	2:M:28:ARG:HH11	1.76	0.50
2:M:428:ARG:HA	2:M:450:GLY:HA3	1.94	0.50
3:D:933:ALA:O	3:D:937:TYR:HD1	1.94	0.50
2:M:728:HIS:O	2:M:729:LEU:HD22	2.12	0.50
3:D:1351:GLU:OE1	3:D:1351:GLU:HA	2.11	0.50
3:N:65:ARG:CD	3:N:66:GLN:H	2.25	0.50
2:M:264:PRO:HB2	2:M:289:THR:CB	2.41	0.50
3:N:81:THR:HB	3:N:85:VAL:HG21	1.91	0.50
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.41	0.50
2:M:478:VAL:HA	2:M:506:ASN:O	2.12	0.50
9:D:2101:HOH:O	4:E:48:MET:HG3	2.11	0.50
2:C:266:ARG:HG3	2:C:266:ARG:HH11	1.77	0.50
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.50
2:M:769:PRO:HD2	9:M:9815:HOH:O	2.11	0.50
2:C:604:ALA:HB3	2:C:612:VAL:O	2.12	0.50
1:A:41:ARG:NH1	1:A:177:VAL:HB	2.25	0.50
1:A:111:ALA:HB3	1:A:124:ASN:O	2.12	0.50
1:A:156:HIS:H	1:A:156:HIS:CD2	2.29	0.50
3:D:630:VAL:HG12	3:D:631:ILE:N	2.27	0.50
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.94	0.50
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.42	0.50
1:B:60:ASP:HB2	9:B:9588:HOH:O	2.11	0.50
2:C:958:THR:HB	9:C:9980:HOH:O	2.11	0.50
3:N:2:LYS:HG2	3:N:3:LYS:HZ2	1.76	0.50
2:M:456:ALA:HA	2:M:541:SER:HA	1.93	0.50
2:M:564:MET:HA	9:M:9338:HOH:O	2.11	0.50
1:K:151:VAL:HG22	9:K:3152:HOH:O	2.11	0.50
3:N:1124:GLN:OE1	3:N:1135:ARG:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:669:GLY:O	2:C:670:GLN:HG3	2.12	0.50
3:N:112:ILE:HD11	3:N:124:GLU:CD	2.32	0.50
3:N:714:GLN:HE22	3:N:732:VAL:HB	1.77	0.50
3:D:399:ARG:HB3	3:D:402:PRO:HG3	1.92	0.50
5:F:209:PHE:HA	5:F:212:LEU:HD12	1.93	0.50
5:F:392:VAL:HG13	9:F:9894:HOH:O	2.10	0.50
1:A:184:THR:O	1:A:192:LEU:HD12	2.11	0.50
2:M:876:VAL:H	2:M:877:PRO:HD2	1.75	0.50
3:N:958:GLU:HB3	9:N:9999:HOH:O	2.10	0.50
3:N:1123:PHE:CE1	3:N:1134:LEU:HG	2.46	0.50
2:C:644:VAL:HB	9:C:2682:HOH:O	2.12	0.50
2:C:770:GLU:HG2	9:D:9612:HOH:O	2.11	0.50
3:D:939:PHE:O	3:D:942:SER:HB3	2.12	0.50
2:C:19:THR:HG21	2:C:124:ASP:O	2.11	0.50
3:D:1409:ALA:HB2	9:D:2109:HOH:O	2.11	0.50
2:C:514:VAL:HG22	9:C:9943:HOH:O	2.11	0.50
3:D:969:ARG:HA	9:D:2563:HOH:O	2.11	0.50
1:B:195:LEU:HD12	1:B:196:THR:N	2.27	0.50
3:N:827:ILE:HG23	9:N:9636:HOH:O	2.12	0.50
2:M:875:GLY:O	2:M:879:ARG:HD3	2.12	0.50
3:N:1103:HIS:HD2	3:N:1462:LEU:H	1.58	0.50
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.93	0.50
1:A:115:LEU:O	1:A:115:LEU:HD12	2.11	0.50
2:M:792:VAL:N	9:M:9305:HOH:O	2.44	0.50
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.27	0.50
3:D:1319:VAL:HA	3:D:1323:GLN:OE1	2.12	0.50
3:N:1349:VAL:HG22	3:N:1372:VAL:HG21	1.94	0.50
2:C:607:ASP:C	2:C:609:ASN:H	2.15	0.50
1:B:90:LEU:HD23	1:B:91:ASN:HD22	1.77	0.50
1:A:182:GLU:O	1:A:194:LYS:HB3	2.11	0.50
3:N:73:CYS:HB3	3:N:76:CYS:O	2.11	0.50
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.77	0.50
5:F:340:SER:O	5:F:342:VAL:N	2.45	0.50
3:N:1335:LEU:HD11	9:N:2029:HOH:O	2.11	0.50
5:P:278:LEU:HB3	5:P:286:PRO:CG	2.27	0.50
2:M:139:GLN:HB3	2:M:334:ARG:HB2	1.93	0.50
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.93	0.50
2:M:649:VAL:HA	2:M:650:ARG:HH21	1.77	0.50
3:N:521:PRO:O	3:N:525:ARG:HG2	2.12	0.50
2:M:110:GLU:HB3	9:M:9372:HOH:O	2.12	0.50
2:M:476:GLY:C	2:M:478:VAL:H	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:LYS:HZ1	1:L:224:TYR:HE1	1.60	0.50
2:C:289:THR:O	2:C:291:ALA:N	2.44	0.50
2:C:759:THR:HG21	2:C:783:ARG:CZ	2.42	0.50
3:D:676:MET:HG3	9:D:9957:HOH:O	2.11	0.50
1:L:36:LEU:O	1:L:39:PRO:HD2	2.12	0.50
3:D:563:PRO:HB3	9:F:9576:HOH:O	2.11	0.50
3:N:956:ILE:HG12	3:N:1039:CYS:O	2.11	0.50
3:N:1124:GLN:HB2	9:N:9329:HOH:O	2.12	0.50
3:D:115:LEU:CD1	3:D:499:VAL:HG22	2.42	0.50
5:P:147:LEU:H	5:P:147:LEU:HD12	1.77	0.50
3:D:894:LYS:HA	9:D:2557:HOH:O	2.11	0.50
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.47	0.50
3:N:844:ALA:O	3:N:867:ARG:HB3	2.11	0.50
3:D:1101:VAL:HG21	3:D:1424:VAL:HG13	1.93	0.50
2:M:139:GLN:OE1	2:M:415:PRO:HD2	2.12	0.50
3:D:6:ARG:HB3	3:D:6:ARG:CZ	2.42	0.50
2:M:304:LEU:HB2	9:M:9883:HOH:O	2.11	0.50
5:F:372:ARG:HB3	9:F:2056:HOH:O	2.12	0.50
3:N:813:LEU:HD23	9:N:9996:HOH:O	2.10	0.50
2:C:260:LEU:HA	2:C:291:ALA:CB	2.41	0.50
3:D:959:GLU:HG3	3:D:1006:ALA:HB1	1.93	0.50
2:M:64:LEU:HD13	9:M:9296:HOH:O	2.12	0.50
5:P:261:PRO:HD3	9:P:8018:HOH:O	2.12	0.50
3:N:599:PRO:HD2	9:N:9833:HOH:O	2.12	0.50
2:C:45:GLN:HB2	2:C:71:TYR:CE2	2.47	0.50
3:N:129:PHE:O	3:N:572:ARG:HG3	2.11	0.50
1:K:7:LYS:NZ	1:K:27:PRO:HG2	2.27	0.50
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.47	0.50
3:N:681:ARG:HB2	3:N:681:ARG:HH11	1.77	0.50
2:C:747:ALA:O	2:C:800:VAL:HG23	2.12	0.50
3:D:1362:LYS:HG3	9:D:2173:HOH:O	2.12	0.50
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.93	0.50
2:M:390:GLN:HA	9:P:4407:HOH:O	2.10	0.50
5:P:215:GLU:O	5:P:218:GLN:HB3	2.11	0.50
2:C:1059:ASP:HB2	9:C:9720:HOH:O	2.12	0.49
3:D:497:GLU:HB2	9:D:2123:HOH:O	2.11	0.49
4:O:45:ARG:HB3	4:O:46:PRO:HD2	1.92	0.49
3:N:1378:TYR:OH	3:N:1431:THR:HA	2.12	0.49
2:M:164:PRO:HD2	2:M:170:PRO:O	2.12	0.49
3:N:1079:LYS:HG3	3:N:1080:GLY:N	2.26	0.49
2:M:48:PHE:HA	9:M:9688:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:321:ILE:HD11	5:P:329:TYR:CB	2.39	0.49
5:P:393:THR:O	5:P:397:ILE:HG13	2.11	0.49
1:L:111:ALA:HB3	1:L:124:ASN:O	2.12	0.49
3:D:864:VAL:HA	9:D:9613:HOH:O	2.11	0.49
1:A:153:ALA:HA	1:A:156:HIS:CD2	2.47	0.49
5:F:158:GLU:HA	5:F:161:GLN:NE2	2.27	0.49
3:N:3:LYS:HA	9:N:2915:HOH:O	2.12	0.49
2:C:479:VAL:HG21	2:C:503:LEU:HD21	1.93	0.49
3:D:166:GLN:HB3	3:D:395:VAL:HG21	1.94	0.49
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.93	0.49
5:P:422:LEU:H	5:P:422:LEU:HD12	1.77	0.49
3:N:502:PHE:CD1	3:N:509:PRO:HB3	2.47	0.49
5:F:277:GLN:HA	9:F:9672:HOH:O	2.11	0.49
1:B:189:ARG:HD2	9:B:9618:HOH:O	2.11	0.49
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.92	0.49
2:C:769:PRO:HA	9:C:9981:HOH:O	2.12	0.49
3:D:67:ARG:HE	3:D:67:ARG:HA	1.76	0.49
2:C:295:ASP:C	2:C:297:GLU:H	2.15	0.49
5:P:119:ILE:HG12	9:P:2011:HOH:O	2.11	0.49
3:D:1263:PHE:HA	3:D:1375:MET:HE2	1.93	0.49
4:O:40:LEU:HD11	4:O:67:GLU:HG2	1.94	0.49
3:N:65:ARG:HB2	5:P:375:LEU:O	2.12	0.49
3:N:507:ASN:HB2	9:N:9257:HOH:O	2.12	0.49
3:D:474:GLU:O	3:D:478:LEU:HG	2.12	0.49
3:D:169:TYR:N	3:D:170:PRO:HD3	2.27	0.49
3:D:127:LEU:HD12	3:D:457:GLY:H	1.77	0.49
3:N:87:ARG:HG3	3:N:524:LEU:HG	1.93	0.49
5:F:273:ARG:HD3	9:F:9638:HOH:O	2.12	0.49
3:N:455:ARG:HH22	5:P:140:ARG:CB	2.25	0.49
3:N:1189:ARG:HB3	3:N:1189:ARG:CZ	2.43	0.49
2:M:606:VAL:HG21	2:M:645:VAL:HG22	1.95	0.49
2:C:86:LYS:CG	2:C:813:VAL:HG12	2.39	0.49
4:E:41:GLU:CA	4:E:45:ARG:HG3	2.42	0.49
2:C:148:PHE:CE1	2:C:281:LEU:HD22	2.47	0.49
3:D:629:SER:HA	9:D:2061:HOH:O	2.12	0.49
1:L:161:ARG:HB3	9:L:4752:HOH:O	2.12	0.49
2:M:346:VAL:HG12	2:M:350:ARG:HE	1.77	0.49
3:D:1274:ILE:O	3:D:1274:ILE:HD12	2.13	0.49
3:N:180:LYS:HG3	9:N:9302:HOH:O	2.11	0.49
2:C:350:ARG:HB3	9:C:2086:HOH:O	2.12	0.49
3:N:966:GLU:O	3:N:969:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:HG12	2:C:990:GLY:O	2.12	0.49
1:L:145:ASP:HB3	9:L:7895:HOH:O	2.12	0.49
2:C:786:LYS:HG3	9:C:2781:HOH:O	2.11	0.49
3:D:217:LYS:HA	9:D:9649:HOH:O	2.13	0.49
3:D:405:ASP:OD1	3:D:407:VAL:HG23	2.13	0.49
5:P:278:LEU:HD13	5:P:290:GLU:HB3	1.95	0.49
3:N:389:GLU:HG2	9:N:9256:HOH:O	2.11	0.49
5:F:160:ASP:HA	5:F:163:LEU:CD1	2.34	0.49
5:P:357:ALA:HB1	5:P:408:LEU:HD11	1.94	0.49
2:C:194:VAL:HG21	2:C:221:LEU:O	2.12	0.49
3:D:172:PRO:HB3	3:D:178:LEU:CB	2.42	0.49
4:O:47:LYS:CA	4:O:54:LEU:HB3	2.42	0.49
1:L:76:VAL:HG23	9:L:2024:HOH:O	2.12	0.49
4:E:24:ALA:O	4:E:28:GLN:HG3	2.12	0.49
3:N:704:ARG:HH12	3:N:743:ASP:CB	2.26	0.49
2:M:259:GLY:HA2	2:M:290:LEU:O	2.12	0.49
5:P:373:LYS:HD3	5:P:378:GLY:C	2.32	0.49
5:F:125:ASP:HA	9:F:9581:HOH:O	2.12	0.49
1:K:62:LEU:HD22	2:M:745:ILE:HB	1.94	0.49
1:K:229:GLN:HB2	9:K:5388:HOH:O	2.10	0.49
2:M:246:ASP:HB3	9:M:9919:HOH:O	2.12	0.49
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.94	0.49
1:L:54:THR:HG21	1:L:143:ARG:NH2	2.26	0.49
3:D:147:VAL:HA	9:D:9668:HOH:O	2.11	0.49
1:L:114:PHE:HB3	9:L:6216:HOH:O	2.11	0.49
5:P:172:ARG:O	5:P:176:ILE:HG13	2.11	0.49
2:M:42:VAL:HG22	2:M:268:ASP:OD2	2.13	0.49
1:L:163:ASN:HA	9:L:5364:HOH:O	2.12	0.49
2:M:9:ILE:CD1	2:M:536:PRO:HD3	2.43	0.49
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.39	0.49
3:D:795:VAL:CG1	3:D:863:VAL:HG22	2.42	0.49
2:M:193:LEU:O	2:M:193:LEU:HD13	2.13	0.49
2:C:266:ARG:HB2	2:C:288:ARG:NE	2.27	0.49
2:C:727:PRO:HG2	2:C:785:VAL:HG12	1.93	0.49
3:N:165:LYS:HB2	3:N:395:VAL:HG11	1.93	0.49
2:M:958:THR:HG23	2:M:961:GLU:HG3	1.93	0.49
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.41	0.49
1:A:30:ARG:HH22	1:B:155:LYS:HZ2	1.60	0.49
3:N:1092:GLY:O	3:N:1096:ARG:N	2.45	0.49
3:D:1366:LYS:HA	3:D:1369:GLU:OE1	2.11	0.49
2:M:452:ILE:HG12	9:M:9712:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:769:PRO:HB2	9:D:9612:HOH:O	2.12	0.49
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.94	0.49
3:N:1110:ALA:HB1	9:N:9774:HOH:O	2.11	0.49
2:C:394:PHE:HB3	9:C:9833:HOH:O	2.12	0.49
2:C:919:ALA:HB2	9:C:9756:HOH:O	2.12	0.49
2:C:590:ASP:HA	9:C:9671:HOH:O	2.11	0.49
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.42	0.49
2:C:627:ARG:N	2:C:627:ARG:HE	1.89	0.49
3:N:9:ARG:HA	3:N:1455:LYS:O	2.12	0.49
3:N:131:LYS:HB2	3:N:456:MET:HE2	1.94	0.49
2:M:313:LEU:HD12	9:M:2079:HOH:O	2.11	0.49
3:D:177:ALA:HA	3:D:199:LEU:HD13	1.94	0.49
5:F:299:TRP:HD1	9:F:9664:HOH:O	1.95	0.49
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.95	0.49
2:M:98:LEU:O	2:M:109:LYS:HG3	2.13	0.49
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.13	0.49
3:D:868:TYR:H	3:D:873:LEU:HD11	1.77	0.49
1:K:91:ASN:O	1:K:94:LEU:HD12	2.13	0.49
3:D:935:LYS:HZ3	3:D:936:TYR:N	2.10	0.49
1:L:109:VAL:HG23	1:L:132:LEU:HD13	1.94	0.49
2:M:720:GLU:HB3	9:M:9349:HOH:O	2.11	0.49
3:N:581:LEU:HD12	3:N:582:LEU:N	2.27	0.49
3:N:112:ILE:HD11	3:N:124:GLU:HG2	1.93	0.49
1:A:184:THR:HG22	1:A:192:LEU:O	2.12	0.49
3:D:902:LEU:HD23	3:D:902:LEU:H	1.78	0.49
3:D:413:ASP:HA	9:D:2284:HOH:O	2.12	0.49
3:D:486:ARG:O	3:D:489:ARG:HG2	2.12	0.49
2:M:777:ILE:HG22	2:M:778:PHE:HD1	1.76	0.49
2:M:332:ARG:HG2	2:M:333:ILE:N	2.27	0.49
2:C:1115:LEU:HD23	3:D:85:VAL:CG1	2.40	0.49
3:D:181:ASP:O	3:D:185:VAL:HG23	2.13	0.49
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.94	0.49
3:N:135:LEU:HD13	3:N:147:VAL:HG12	1.94	0.49
2:C:28:ARG:HA	9:C:2297:HOH:O	2.12	0.49
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.47	0.49
1:L:45:LEU:HD21	1:L:177:VAL:HG23	1.94	0.49
2:M:644:VAL:HB	9:M:9422:HOH:O	2.12	0.49
2:C:327:HIS:HB3	2:C:330:ASN:ND2	2.28	0.49
3:N:401:TYR:N	3:N:402:PRO:HD3	2.28	0.49
2:C:40:GLU:HG2	9:C:2473:HOH:O	2.13	0.49
3:D:1379:VAL:N	9:D:2424:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.42	0.49
2:M:897:LEU:HB3	2:M:899:GLN:NE2	2.28	0.49
2:C:602:GLU:HB3	9:C:9979:HOH:O	2.12	0.49
1:K:206:THR:CG2	1:K:209:GLU:H	2.24	0.49
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.94	0.49
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.13	0.49
3:D:1499:ARG:HA	9:D:2938:HOH:O	2.11	0.49
3:D:1303:TYR:HA	9:D:2028:HOH:O	2.13	0.49
3:D:710:ARG:NH1	3:D:710:ARG:HG2	2.25	0.49
3:N:26:VAL:N	9:N:9259:HOH:O	2.44	0.49
5:F:266:GLU:HA	5:F:269:ASN:ND2	2.24	0.49
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.47	0.49
2:M:583:LEU:O	2:M:587:VAL:HG23	2.13	0.49
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.12	0.49
2:M:101:ILE:HG22	2:M:102:HIS:N	2.26	0.49
1:L:41:ARG:HG3	1:L:177:VAL:HB	1.94	0.49
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.94	0.49
1:B:162:ILE:HB	9:B:9818:HOH:O	2.11	0.49
1:K:198:ARG:HD3	1:K:200:TRP:CH2	2.48	0.49
2:C:1035:MET:HB3	3:D:707:THR:HB	1.94	0.49
1:K:184:THR:O	1:K:192:LEU:HB2	2.12	0.49
3:D:1159:ARG:HH11	3:D:1159:ARG:HG3	1.76	0.49
2:C:744:ARG:HA	9:C:9595:HOH:O	2.13	0.49
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.94	0.49
5:F:169:GLU:HA	9:F:9835:HOH:O	2.11	0.49
2:M:1028:GLY:HA2	9:M:9259:HOH:O	2.12	0.49
3:N:153:LEU:HD22	9:N:2799:HOH:O	2.11	0.49
2:M:82:GLU:HG3	9:M:9567:HOH:O	2.13	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.43	0.49
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.12	0.49
2:M:269:LEU:HD22	2:M:288:ARG:HB2	1.94	0.49
3:N:412:GLY:O	3:N:421:LEU:HB3	2.12	0.49
3:D:179:VAL:CG2	3:D:389:GLU:HG3	2.42	0.49
2:C:689:VAL:HG21	2:C:870:ILE:HB	1.93	0.49
4:E:25:LYS:O	4:E:28:GLN:HB2	2.13	0.49
2:M:545:ASN:HB3	2:M:583:LEU:HD12	1.95	0.49
2:C:1102:LEU:HD11	9:D:9712:HOH:O	2.13	0.49
1:K:11:PHE:HB2	9:K:3188:HOH:O	2.12	0.49
5:F:350:LEU:O	5:F:354:LEU:HG	2.13	0.49
2:M:776:SER:HA	2:M:780:GLU:CB	2.41	0.49
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.13	0.49
9:N:2509:HOH:O	5:P:94:LEU:HD21	2.13	0.49
3:D:1310:ARG:HB3	9:D:9775:HOH:O	2.13	0.49
3:N:968:ASP:O	3:N:971:LEU:HB3	2.12	0.49
3:N:947:ILE:HD12	3:N:947:ILE:O	2.12	0.49
3:N:657:LEU:HD22	3:N:691:LEU:HD13	1.93	0.49
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.95	0.49
3:N:1448:THR:O	3:N:1451:ALA:HB3	2.13	0.49
5:P:320:PRO:HB3	9:P:5311:HOH:O	2.12	0.49
5:P:277:GLN:HG2	9:P:1413:HOH:O	2.12	0.49
5:F:395:GLU:O	5:F:399:GLN:HB2	2.12	0.49
4:O:25:LYS:O	4:O:28:GLN:HB2	2.13	0.49
2:M:222:MET:HG3	9:M:2024:HOH:O	2.13	0.49
1:L:101:LEU:HA	9:L:1474:HOH:O	2.13	0.49
3:N:168:THR:OG1	3:N:393:ILE:HB	2.11	0.49
4:O:63:TRP:O	4:O:67:GLU:HG3	2.13	0.49
2:M:42:VAL:HA	2:M:46:ALA:HB2	1.95	0.49
3:D:89:ARG:O	3:D:521:PRO:HG3	2.13	0.49
3:D:116:LEU:O	3:D:118:LEU:N	2.45	0.49
2:M:472:ARG:HE	2:M:532:MET:HE2	1.77	0.49
2:C:564:MET:HG2	2:C:840:ALA:HB3	1.95	0.49
1:B:195:LEU:HD12	1:B:196:THR:H	1.76	0.49
3:N:1330:ILE:HG12	9:N:9950:HOH:O	2.13	0.49
3:N:1442:ASN:HD22	3:N:1442:ASN:H	1.60	0.49
1:L:132:LEU:HG	9:L:2881:HOH:O	2.12	0.49
1:K:182:GLU:O	1:K:194:LYS:HB3	2.12	0.49
5:P:76:SER:O	5:P:80:PRO:HD2	2.12	0.49
2:C:446:GLY:HA3	9:C:9687:HOH:O	2.12	0.49
1:B:184:THR:HG22	1:B:192:LEU:O	2.11	0.49
3:D:1012:GLU:HB3	9:D:9868:HOH:O	2.13	0.49
2:C:27:ARG:HH11	2:C:27:ARG:HG3	1.77	0.49
5:P:168:LYS:HG3	9:P:3066:HOH:O	2.12	0.49
2:M:956:GLY:HA2	9:M:2324:HOH:O	2.12	0.49
5:F:162:LYS:HE3	9:F:9869:HOH:O	2.13	0.49
2:C:1073:GLY:HA3	3:D:659:LYS:NZ	2.28	0.49
2:C:142:ARG:HG3	9:C:2425:HOH:O	2.11	0.49
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.47	0.49
3:D:1348:LEU:O	3:D:1352:ILE:HG13	2.13	0.49
5:P:375:LEU:HG	9:P:3218:HOH:O	2.13	0.49
3:D:1465:ASN:OD1	3:D:1470:ARG:HB3	2.12	0.49
2:M:288:ARG:HB3	9:M:9500:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.94	0.49
2:M:841:ASN:OD1	2:M:843:HIS:HB2	2.13	0.49
3:N:141:ILE:H	3:N:141:ILE:CD1	2.24	0.49
1:L:62:LEU:H	1:L:62:LEU:HD12	1.78	0.49
2:M:696:LYS:HA	9:M:9665:HOH:O	2.12	0.49
3:D:661:MET:CE	3:D:673:ALA:HB1	2.42	0.49
5:F:419:ARG:HH11	5:F:419:ARG:HG2	1.76	0.49
4:E:30:LEU:O	4:E:35:PHE:HA	2.12	0.49
1:A:45:LEU:HD21	1:A:177:VAL:HG23	1.93	0.49
1:B:48:ILE:HG23	9:B:9710:HOH:O	2.12	0.49
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.95	0.49
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.95	0.49
5:P:198:ILE:HG12	5:P:244:ARG:HH12	1.78	0.49
2:C:144:PRO:C	2:C:276:LYS:HZ2	2.16	0.49
1:A:94:LEU:HD21	1:A:119:ASP:HB2	1.94	0.49
5:P:77:THR:O	5:P:80:PRO:HG2	2.13	0.49
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.94	0.49
2:C:84:ARG:HH11	2:C:84:ARG:HG3	1.77	0.49
3:N:1437:ALA:HB2	9:N:9283:HOH:O	2.11	0.49
2:C:595:LEU:CD1	2:C:639:GLN:HG2	2.43	0.49
2:M:657:ASP:HB3	2:M:661:SER:OG	2.13	0.49
3:N:1282:ARG:HG2	9:N:9906:HOH:O	2.12	0.49
3:D:1247:ALA:HB1	9:D:2742:HOH:O	2.13	0.49
3:N:1287:GLU:HA	9:N:9764:HOH:O	2.12	0.49
3:N:413:ASP:OD2	3:N:419:ASP:HA	2.13	0.49
3:D:1304:LYS:N	3:D:1304:LYS:HD3	2.16	0.48
2:M:144:PRO:HA	2:M:163:ILE:O	2.13	0.48
1:A:34:VAL:HA	9:A:9604:HOH:O	2.12	0.48
2:M:100:LEU:HG	2:M:368:THR:HG23	1.94	0.48
3:D:1336:LEU:HD13	3:D:1376:MET:HE1	1.95	0.48
3:N:1120:VAL:HA	3:N:1346:ARG:HH22	1.78	0.48
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.47	0.48
2:M:534:VAL:H	2:M:538:GLN:NE2	2.11	0.48
2:M:254:VAL:HG12	9:M:2026:HOH:O	2.12	0.48
3:D:145:VAL:HG21	9:D:9785:HOH:O	2.13	0.48
3:D:729:HIS:ND1	3:D:730:PRO:N	2.61	0.48
1:B:162:ILE:HG13	9:B:9680:HOH:O	2.13	0.48
3:D:1148:VAL:HG11	3:D:1203:LYS:HD2	1.95	0.48
2:M:575:GLN:HG2	2:M:671:ASN:ND2	2.27	0.48
2:M:570:PRO:HB3	2:M:660:ALA:HB2	1.94	0.48
1:K:186:LEU:HB2	1:K:192:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:9359:HOH:O	4:O:50:THR:HG21	2.12	0.48
2:C:216:GLU:H	2:C:216:GLU:CD	2.16	0.48
3:N:1282:ARG:HB2	3:N:1293:PHE:HB2	1.95	0.48
2:C:877:PRO:HB3	3:D:1020:LEU:CD1	2.43	0.48
2:M:269:LEU:HB3	9:M:9569:HOH:O	2.13	0.48
3:D:169:TYR:CG	3:D:169:TYR:O	2.67	0.48
3:N:422:ALA:H	3:N:427:VAL:HG11	1.77	0.48
3:N:493:ARG:NH2	3:N:1389:LEU:HD11	2.28	0.48
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.12	0.48
5:F:115:LYS:HD3	5:F:173:TYR:CE2	2.48	0.48
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.48	0.48
2:C:574:ALA:O	2:C:575:GLN:HB2	2.12	0.48
1:B:23:PHE:O	1:B:196:THR:HA	2.12	0.48
3:D:873:LEU:HA	9:D:2884:HOH:O	2.12	0.48
3:N:863:VAL:HG12	9:N:9938:HOH:O	2.12	0.48
1:L:119:ASP:HB3	9:L:1485:HOH:O	2.12	0.48
3:N:704:ARG:HH12	3:N:743:ASP:CG	2.16	0.48
2:C:164:PRO:HD2	2:C:170:PRO:O	2.13	0.48
2:C:266:ARG:O	2:C:288:ARG:HD3	2.13	0.48
5:P:185:GLN:O	5:P:189:GLU:HG3	2.13	0.48
2:C:428:ARG:HA	2:C:450:GLY:HA3	1.94	0.48
2:M:736:ASP:HA	2:M:744:ARG:NH1	2.28	0.48
3:N:1049:SER:OG	3:N:1051:GLU:HG2	2.14	0.48
5:F:139:ALA:HB1	5:F:152:ASP:HB3	1.94	0.48
1:L:229:GLN:HG2	9:L:6318:HOH:O	2.13	0.48
3:D:235:ALA:HB1	9:D:9573:HOH:O	2.13	0.48
2:M:446:GLY:O	2:M:449:ILE:HG13	2.12	0.48
4:E:8:LYS:HD3	9:E:9637:HOH:O	2.13	0.48
1:B:159:LYS:HE3	9:B:9720:HOH:O	2.14	0.48
3:D:786:ILE:HD13	3:D:1027:GLY:HA3	1.94	0.48
5:F:300:ASP:HB2	9:F:9768:HOH:O	2.13	0.48
2:M:343:GLN:HB2	9:M:2031:HOH:O	2.13	0.48
2:C:42:VAL:HG12	2:C:43:GLY:N	2.24	0.48
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.42	0.48
9:C:2198:HOH:O	5:F:350:LEU:HD21	2.12	0.48
3:N:959:GLU:HG3	3:N:1006:ALA:HB1	1.95	0.48
5:F:371:LEU:HA	5:F:375:LEU:HB2	1.95	0.48
2:C:722:ILE:HG22	9:C:2273:HOH:O	2.13	0.48
2:M:189:ARG:HH21	2:M:243:ARG:CZ	2.26	0.48
3:D:754:PHE:O	3:D:757:ALA:HB3	2.13	0.48
3:N:55:ASP:HA	3:N:82:LYS:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:PHE:CE2	5:F:283:GLY:HA3	2.48	0.48
2:M:549:PHE:HB3	2:M:552:HIS:CD2	2.48	0.48
2:M:261:ILE:CG2	2:M:262:ALA:H	2.26	0.48
3:N:1087:ARG:HE	3:N:1238:MET:HB2	1.77	0.48
3:N:1276:GLU:HG3	3:N:1303:TYR:OH	2.13	0.48
3:D:618:LEU:HD21	9:D:2041:HOH:O	2.14	0.48
3:N:869:MET:HA	9:N:2163:HOH:O	2.14	0.48
1:K:65:PHE:HE1	2:M:799:ILE:HD11	1.78	0.48
2:M:1065:ALA:HB1	2:M:1077:PRO:HG2	1.96	0.48
2:M:631:SER:HG	2:M:635:THR:N	2.11	0.48
3:D:649:ALA:CB	3:D:691:LEU:HD21	2.43	0.48
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.95	0.48
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.13	0.48
3:N:829:VAL:HB	9:N:9280:HOH:O	2.12	0.48
2:M:48:PHE:CD2	2:M:52:PHE:HE2	2.31	0.48
2:M:52:PHE:HE1	2:M:98:LEU:HD21	1.78	0.48
5:P:155:THR:O	5:P:159:ILE:HG13	2.14	0.48
4:E:23:VAL:HG23	4:E:64:ALA:HB3	1.94	0.48
3:N:1382:THR:HA	9:N:9517:HOH:O	2.12	0.48
3:N:416:ALA:H	3:N:417:PRO:CD	2.26	0.48
3:D:1058:ARG:HG3	3:D:1058:ARG:NH1	2.28	0.48
5:P:288:TYR:H	5:P:288:TYR:HD1	1.60	0.48
4:O:50:THR:HG23	9:O:1048:HOH:O	2.13	0.48
2:C:807:ARG:HD2	9:C:2355:HOH:O	2.12	0.48
2:M:226:VAL:HG13	2:M:227:PHE:CD2	2.48	0.48
2:M:753:ASP:HA	3:N:679:ARG:HD2	1.95	0.48
2:M:722:ILE:HG21	2:M:821:GLU:OE2	2.13	0.48
1:B:1:MET:O	1:B:6:LEU:HD22	2.13	0.48
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.95	0.48
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.48	0.48
5:F:169:GLU:CD	5:F:169:GLU:H	2.15	0.48
3:N:557:LEU:HD11	9:P:1239:HOH:O	2.13	0.48
3:D:1463:LYS:HG2	9:D:2672:HOH:O	2.12	0.48
2:C:572:ILE:HD11	2:C:698:ASP:HB3	1.94	0.48
3:D:2:LYS:HB3	9:D:9972:HOH:O	2.12	0.48
3:N:1058:ARG:HG2	9:N:9994:HOH:O	2.12	0.48
3:D:1117:TYR:HB3	9:D:9720:HOH:O	2.12	0.48
3:D:984:THR:HG22	3:D:987:GLU:H	1.79	0.48
4:O:45:ARG:HA	9:O:6351:HOH:O	2.13	0.48
2:M:165:LEU:HD22	9:M:9925:HOH:O	2.13	0.48
2:M:149:THR:HG22	9:M:9475:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:163:LEU:HD13	5:P:174:LEU:CD2	2.43	0.48
5:F:271:LEU:HD21	5:F:299:TRP:CZ3	2.48	0.48
2:C:803:THR:HG22	2:C:825:VAL:HG22	1.95	0.48
2:M:597:ALA:HA	9:M:9794:HOH:O	2.13	0.48
3:N:860:LEU:HB2	3:N:861:GLN:HE22	1.77	0.48
3:N:1147:ARG:HD2	3:N:1188:VAL:HG21	1.95	0.48
3:N:64:LYS:HZ3	5:P:377:ASP:HA	1.78	0.48
2:M:643:VAL:HG23	9:M:9275:HOH:O	2.12	0.48
3:N:1440:PHE:O	3:N:1443:THR:HG23	2.13	0.48
5:P:94:LEU:HB3	5:P:98:GLU:HB2	1.95	0.48
2:M:455:LEU:HD22	2:M:459:ALA:CB	2.44	0.48
2:C:204:GLN:HA	9:C:9805:HOH:O	2.12	0.48
1:K:227:ASN:ND2	1:K:227:ASN:H	2.12	0.48
3:D:1413:THR:HA	9:D:9958:HOH:O	2.12	0.48
5:P:147:LEU:HD13	9:P:1942:HOH:O	2.13	0.48
3:N:200:ASP:HA	9:N:2149:HOH:O	2.13	0.48
2:M:381:ALA:HB1	9:M:9341:HOH:O	2.12	0.48
3:N:561:GLY:HA3	9:N:9263:HOH:O	2.13	0.48
2:M:551:GLU:H	2:M:551:GLU:CD	2.16	0.48
4:E:14:ASP:HA	9:E:9592:HOH:O	2.13	0.48
2:M:978:ARG:HH11	2:M:978:ARG:HG3	1.79	0.48
3:D:1354:LYS:HA	9:D:2684:HOH:O	2.13	0.48
3:D:1435:LEU:HG	3:D:1467:ILE:HD12	1.95	0.48
3:D:500:ARG:NH2	3:D:1388:ARG:NE	2.57	0.48
2:M:142:ARG:HB2	2:M:163:ILE:HD13	1.95	0.48
3:D:177:ALA:C	3:D:199:LEU:HD13	2.32	0.48
2:M:1067:TYR:HE1	3:N:655:PRO:HG3	1.77	0.48
3:N:861:GLN:N	3:N:861:GLN:CD	2.67	0.48
2:M:490:GLU:O	2:M:493:ARG:HB2	2.14	0.48
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.96	0.48
5:P:96:LEU:HD12	9:P:1515:HOH:O	2.12	0.48
3:D:1314:LYS:HD3	3:D:1314:LYS:H	1.77	0.48
3:D:1188:VAL:HG11	9:D:9650:HOH:O	2.14	0.48
3:D:149:LYS:HB3	9:D:2253:HOH:O	2.13	0.48
3:N:2:LYS:HG2	3:N:3:LYS:NZ	2.28	0.48
3:N:1047:LYS:HD2	3:N:1051:GLU:HG3	1.95	0.48
2:C:683:ASN:OD1	2:C:872:ASN:HB2	2.14	0.48
1:L:6:LEU:C	1:L:8:ALA:H	2.17	0.48
3:N:962:GLN:O	3:N:966:GLU:HG3	2.14	0.48
3:N:549:ASN:ND2	5:P:254:GLN:NE2	2.62	0.48
3:N:500:ARG:HH11	3:N:500:ARG:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:218:LYS:N	9:D:9726:HOH:O	2.45	0.48
3:D:845:ASN:O	3:D:848:GLU:HB2	2.14	0.48
3:D:1038:LEU:HA	3:D:1061:PHE:HB2	1.95	0.48
3:D:699:VAL:H	3:D:756:GLN:HE22	1.62	0.48
3:N:1425:THR:HG22	3:N:1429:LEU:HD22	1.96	0.48
2:M:334:ARG:HB3	9:M:9771:HOH:O	2.12	0.48
2:M:333:ILE:HG22	2:M:465:GLY:HA2	1.95	0.48
2:C:244:PRO:HG2	2:C:246:ASP:OD1	2.13	0.48
3:N:87:ARG:HD2	3:N:524:LEU:HD23	1.96	0.48
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.39	0.48
3:N:1243:THR:O	3:N:1269:LYS:HG3	2.12	0.48
3:N:630:VAL:HG12	3:N:631:ILE:N	2.27	0.48
1:A:143:ARG:CD	1:A:158:ILE:HG21	2.44	0.48
3:D:864:VAL:HG12	3:D:865:THR:N	2.28	0.48
2:M:300:ASP:OD2	2:M:303:PHE:HB2	2.13	0.48
2:C:12:VAL:HA	9:C:2815:HOH:O	2.14	0.48
4:E:40:LEU:O	4:E:40:LEU:HD12	2.13	0.48
3:N:166:GLN:HB3	3:N:395:VAL:CG2	2.43	0.48
5:F:236:SER:HA	9:F:9646:HOH:O	2.14	0.48
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.14	0.48
2:C:341:THR:HG21	9:C:9696:HOH:O	2.13	0.48
1:L:182:GLU:HB2	9:L:8791:HOH:O	2.14	0.48
2:C:87:ASP:HB2	9:C:9712:HOH:O	2.13	0.48
1:B:36:LEU:O	1:B:39:PRO:HD2	2.13	0.48
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.96	0.48
2:C:404:LEU:HD12	2:C:407:LYS:HE2	1.95	0.48
1:L:107:LYS:HB2	9:L:1363:HOH:O	2.14	0.48
5:P:148:LYS:NZ	5:P:148:LYS:HB2	2.28	0.48
2:M:69:LEU:HB2	2:M:97:ARG:CB	2.44	0.48
2:M:295:ASP:C	2:M:297:GLU:H	2.16	0.48
3:D:800:LYS:HE2	3:D:830:ALA:CB	2.43	0.48
3:D:830:ALA:HB1	9:D:2375:HOH:O	2.14	0.48
3:N:1449:GLU:HG3	9:N:9417:HOH:O	2.13	0.48
2:M:712:ALA:HB3	2:M:821:GLU:HG3	1.95	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.44	0.48
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.49	0.48
1:A:65:PHE:CZ	2:C:830:LYS:HG3	2.49	0.48
3:N:588:GLY:HA2	9:N:9647:HOH:O	2.13	0.48
3:D:1114:THR:CG2	3:D:1195:GLN:HB2	2.44	0.48
3:D:1263:PHE:O	3:D:1424:VAL:HG23	2.13	0.48
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:LEU:O	3:D:713:ILE:HA	2.14	0.48
2:M:334:ARG:HD2	9:M:9389:HOH:O	2.13	0.48
3:D:524:LEU:C	3:D:526:PRO:HD3	2.34	0.48
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.94	0.48
3:D:966:GLU:HG3	3:D:969:ARG:NH2	2.28	0.48
5:F:393:THR:HG22	5:F:394:ARG:N	2.27	0.48
5:F:421:PHE:C	5:F:423:ASP:H	2.16	0.48
3:D:54:LYS:HD3	3:D:55:ASP:OD1	2.14	0.48
3:N:813:LEU:HD12	3:N:814:ALA:N	2.29	0.48
1:L:56:VAL:HB	1:L:165:ILE:HD11	1.94	0.48
3:N:959:GLU:HB2	3:N:963:TYR:CE2	2.49	0.48
3:D:162:ARG:HB2	3:D:162:ARG:CZ	2.43	0.48
3:D:162:ARG:HB3	9:D:9697:HOH:O	2.13	0.48
2:M:769:PRO:HD3	9:M:2572:HOH:O	2.13	0.48
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.96	0.48
3:N:1376:MET:HB3	9:N:9377:HOH:O	2.13	0.48
5:P:158:GLU:HA	5:P:161:GLN:HG3	1.95	0.48
1:K:178:ALA:HB2	2:M:864:GLY:H	1.78	0.48
1:K:198:ARG:HD3	1:K:200:TRP:HH2	1.79	0.48
2:C:958:THR:HG23	2:C:961:GLU:H	1.78	0.48
2:M:929:ARG:NH2	9:M:2113:HOH:O	2.45	0.48
3:N:502:PHE:CE2	3:N:1452:ILE:HG13	2.49	0.48
1:A:127:LEU:HD12	1:A:128:HIS:N	2.29	0.48
3:N:202:VAL:HG11	9:N:9932:HOH:O	2.13	0.48
1:K:183:ASP:OD1	2:M:938:LYS:HE3	2.14	0.48
2:C:443:THR:HG21	3:D:1078:ARG:HE	1.78	0.48
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.44	0.48
3:D:556:LYS:HB3	9:F:9588:HOH:O	2.12	0.48
3:D:18:ILE:HD12	3:D:518:PRO:HG3	1.96	0.48
3:N:1046:GLN:N	9:N:9308:HOH:O	2.43	0.48
5:F:299:TRP:CD2	5:F:303:ARG:HD3	2.49	0.48
2:C:92:ALA:O	2:C:118:ILE:HD13	2.14	0.48
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.96	0.48
2:M:983:ILE:HD12	2:M:987:ILE:HD12	1.94	0.48
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.95	0.48
5:P:416:ARG:NH1	5:P:419:ARG:HD3	2.29	0.48
1:K:89:PHE:HZ	1:K:144:VAL:HG12	1.79	0.48
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.95	0.48
1:K:6:LEU:C	1:K:8:ALA:H	2.17	0.48
5:F:80:PRO:HA	5:F:83:GLN:HB3	1.94	0.48
2:M:190:LYS:NZ	9:M:9816:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:142:LEU:HA	9:N:9368:HOH:O	2.14	0.48
3:D:988:ARG:HB3	9:D:9919:HOH:O	2.14	0.48
3:N:137:PRO:HB2	9:N:9902:HOH:O	2.13	0.48
2:M:1004:LYS:HE3	2:M:1027:PHE:CE1	2.48	0.48
3:D:1339:LYS:HD2	9:D:2575:HOH:O	2.14	0.48
2:C:882:LEU:HD12	3:D:1061:PHE:HB3	1.95	0.48
3:N:1478:SER:C	3:N:1480:PHE:N	2.67	0.48
3:N:181:ASP:O	3:N:185:VAL:HG23	2.14	0.48
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.95	0.48
2:M:892:LEU:HD21	2:M:967:PHE:CE1	2.48	0.48
2:C:369:PRO:HG2	2:C:370:ALA:H	1.78	0.48
9:C:9793:HOH:O	3:D:21:TRP:HB3	2.13	0.48
3:N:1380:GLU:HG2	3:N:1381:VAL:N	2.28	0.48
3:D:179:VAL:HG21	9:D:9579:HOH:O	2.13	0.48
3:N:834:THR:HG22	3:N:838:ARG:NE	2.28	0.48
3:D:957:PRO:HG2	3:D:1007:VAL:CA	2.42	0.48
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.44	0.48
1:B:47:SER:O	1:B:49:PRO:N	2.47	0.48
9:A:9662:HOH:O	2:C:645:VAL:HG21	2.14	0.48
2:C:68:PHE:HZ	2:C:71:TYR:HD2	1.61	0.48
3:N:584:ASN:H	3:N:602:SER:HB3	1.79	0.48
1:L:156:HIS:CD2	1:L:158:ILE:HG12	2.49	0.48
2:M:292:ARG:HB2	2:M:299:LYS:NZ	2.28	0.48
2:C:1081:VAL:HB	2:C:1086:ARG:HE	1.79	0.48
5:F:260:ILE:HD11	5:F:264:MET:HB3	1.96	0.48
3:N:1156:LEU:HD23	3:N:1182:GLU:OE1	2.13	0.48
4:E:81:PRO:HA	9:E:9589:HOH:O	2.14	0.48
2:C:1072:LYS:HE2	9:C:2855:HOH:O	2.14	0.48
1:B:220:GLU:HB3	9:B:9783:HOH:O	2.14	0.48
3:N:1415:VAL:HG23	9:N:9894:HOH:O	2.14	0.48
3:N:1168:MET:HE2	9:N:9270:HOH:O	2.14	0.48
2:M:859:PRO:O	2:M:867:VAL:HG22	2.14	0.47
3:D:154:THR:HG22	9:D:9682:HOH:O	2.14	0.47
3:D:86:ARG:HG2	3:D:523:ASP:OD1	2.14	0.47
2:C:1115:LEU:HD22	3:D:88:TYR:CD1	2.47	0.47
3:N:984:THR:HG23	3:N:986:ARG:N	2.29	0.47
2:C:130:ASN:HB3	9:C:9665:HOH:O	2.12	0.47
2:M:67:ASP:HA	9:M:9629:HOH:O	2.12	0.47
2:M:1005:MET:HG2	9:M:9335:HOH:O	2.14	0.47
2:M:397:GLU:H	2:M:633:GLN:HE22	1.62	0.47
3:N:1147:ARG:NH2	9:N:9659:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:795:VAL:HG13	3:D:863:VAL:HG22	1.96	0.47
2:M:302:VAL:O	2:M:306:THR:HG23	2.14	0.47
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.95	0.47
3:N:8:VAL:HG23	9:N:9608:HOH:O	2.13	0.47
3:N:71:LYS:HE3	9:N:2288:HOH:O	2.13	0.47
5:F:220:LEU:O	5:F:224:VAL:HG23	2.13	0.47
2:C:762:LYS:HD3	2:C:771:GLU:OE2	2.13	0.47
3:D:62:LYS:HD3	9:D:2796:HOH:O	2.13	0.47
5:P:352:GLU:HG2	9:P:6518:HOH:O	2.14	0.47
2:C:56:GLU:HG2	9:C:2542:HOH:O	2.13	0.47
3:N:965:GLU:HB3	9:N:9892:HOH:O	2.14	0.47
5:P:400:ILE:HG12	9:P:1779:HOH:O	2.13	0.47
3:N:12:LEU:HB2	9:N:9257:HOH:O	2.13	0.47
2:M:141:HIS:HB2	2:M:418:LEU:HD12	1.94	0.47
2:M:324:ASP:HB3	2:M:327:HIS:CD2	2.40	0.47
5:P:131:VAL:O	5:P:135:ILE:HG12	2.14	0.47
3:D:119:SER:N	3:D:123:LEU:HD13	2.28	0.47
5:F:270:LYS:HE3	9:F:9917:HOH:O	2.13	0.47
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.96	0.47
3:N:907:GLU:O	3:N:911:LEU:HD13	2.13	0.47
3:N:448:GLU:CD	3:N:448:GLU:N	2.67	0.47
2:M:92:ALA:HB1	9:M:9468:HOH:O	2.13	0.47
3:N:706:PRO:HG2	9:N:9369:HOH:O	2.13	0.47
2:M:644:VAL:HG22	2:M:647:GLN:NE2	2.29	0.47
3:N:1435:LEU:HB2	9:N:9646:HOH:O	2.15	0.47
3:D:1133:ARG:NH2	9:D:9997:HOH:O	2.47	0.47
1:B:9:PRO:HB3	1:B:25:LEU:CG	2.44	0.47
3:N:1311:LEU:H	3:N:1311:LEU:CD2	2.24	0.47
2:M:879:ARG:H	2:M:879:ARG:HD2	1.78	0.47
3:D:1036:ARG:HG2	9:D:9667:HOH:O	2.15	0.47
2:C:18:LEU:HD12	2:C:18:LEU:N	2.28	0.47
2:M:503:LEU:HD12	2:M:505:GLY:O	2.14	0.47
1:A:91:ASN:HA	9:A:9714:HOH:O	2.13	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.13	0.47
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.44	0.47
3:N:1197:ARG:HD3	9:N:9581:HOH:O	2.13	0.47
3:D:827:ILE:HG12	9:D:2351:HOH:O	2.14	0.47
3:D:542:ASP:O	3:D:546:ARG:HG2	2.13	0.47
3:N:496:LEU:HG	3:N:500:ARG:HG2	1.96	0.47
4:E:81:PRO:HD3	9:E:9619:HOH:O	2.13	0.47
4:E:96:GLU:HA	9:E:9628:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:920:LEU:HA	9:N:2152:HOH:O	2.13	0.47
2:M:679:PHE:CD1	2:M:870:ILE:HD13	2.48	0.47
3:D:1236:LEU:HD22	3:D:1355:VAL:HG12	1.96	0.47
3:D:983:LEU:HA	3:D:987:GLU:OE2	2.14	0.47
3:D:523:ASP:HB3	9:D:2189:HOH:O	2.13	0.47
2:M:516:ARG:NH2	3:N:1068:LEU:HB2	2.28	0.47
2:M:506:ASN:HB2	9:M:9830:HOH:O	2.13	0.47
2:C:724:ARG:HD3	2:C:740:GLU:HA	1.96	0.47
3:N:1253:THR:HG23	3:N:1258:ARG:HH11	1.79	0.47
3:N:441:ARG:HE	3:N:441:ARG:HA	1.79	0.47
3:D:1493:LYS:HD3	9:D:9925:HOH:O	2.14	0.47
2:C:365:ASP:C	2:C:367:LEU:HD23	2.34	0.47
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.14	0.47
3:D:488:ARG:HB3	3:D:488:ARG:CZ	2.44	0.47
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.44	0.47
2:C:831:ARG:HH21	2:C:999:HIS:HB2	1.78	0.47
3:N:799:LYS:HG2	9:N:9312:HOH:O	2.14	0.47
2:M:926:PHE:O	2:M:929:ARG:HB2	2.14	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.15	0.47
3:N:76:CYS:HA	9:N:9585:HOH:O	2.14	0.47
3:D:894:LYS:O	3:D:898:GLU:HG3	2.13	0.47
1:L:96:THR:HB	1:L:145:ASP:OD2	2.13	0.47
3:N:1191:PRO:HD3	3:N:1204:CYS:O	2.13	0.47
5:P:257:THR:HB	5:P:314:PRO:HG3	1.97	0.47
3:D:1092:GLY:O	3:D:1096:ARG:N	2.42	0.47
2:C:34:VAL:HG22	9:C:9698:HOH:O	2.14	0.47
2:M:965:GLU:HG2	9:M:9258:HOH:O	2.15	0.47
2:M:325:ILE:HG21	9:M:2230:HOH:O	2.15	0.47
2:C:971:LYS:NZ	9:C:9615:HOH:O	2.47	0.47
2:M:313:LEU:HD13	2:M:321:GLU:O	2.15	0.47
3:N:523:ASP:O	3:N:526:PRO:HG3	2.14	0.47
5:F:215:GLU:O	5:F:218:GLN:HB3	2.15	0.47
4:O:47:LYS:O	4:O:54:LEU:HD13	2.14	0.47
4:E:47:LYS:CA	4:E:54:LEU:HB3	2.45	0.47
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.30	0.47
2:M:254:VAL:HG13	2:M:258:TYR:CE1	2.48	0.47
2:C:291:ALA:O	2:C:292:ARG:HB2	2.14	0.47
1:L:169:ALA:HA	9:L:1542:HOH:O	2.15	0.47
4:E:51:LEU:C	4:E:53:GLY:H	2.16	0.47
2:C:721:ARG:HD3	9:C:9781:HOH:O	2.14	0.47
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG21	9:B:9631:HOH:O	2.14	0.47
1:K:173:PRO:HB2	1:K:205:VAL:HG22	1.96	0.47
1:L:115:LEU:HD12	1:L:115:LEU:O	2.14	0.47
5:P:353:GLU:CG	5:P:417:LYS:HB3	2.44	0.47
3:D:1044:LEU:HB2	9:D:2029:HOH:O	2.14	0.47
5:P:209:PHE:CZ	5:P:213:ILE:HD11	2.49	0.47
1:A:140:MET:HA	9:A:9798:HOH:O	2.14	0.47
1:L:8:ALA:HA	9:L:1271:HOH:O	2.14	0.47
5:F:325:LYS:HB2	9:F:9915:HOH:O	2.14	0.47
3:N:1360:GLY:HA3	9:N:9449:HOH:O	2.14	0.47
1:L:201:THR:HG22	1:L:203:GLY:H	1.79	0.47
5:F:104:ARG:HG3	5:F:229:TYR:OH	2.15	0.47
3:N:845:ASN:H	3:N:848:GLU:HG3	1.78	0.47
3:N:74:GLU:HG2	9:N:2213:HOH:O	2.12	0.47
2:C:1105:LYS:O	2:C:1107:ASN:N	2.48	0.47
2:M:607:ASP:C	2:M:609:ASN:H	2.17	0.47
1:L:23:PHE:O	1:L:196:THR:HA	2.13	0.47
3:D:1307:LYS:HG2	9:D:2092:HOH:O	2.14	0.47
9:M:9660:HOH:O	3:N:20:SER:HA	2.13	0.47
4:O:41:GLU:HB3	4:O:42:PRO:HD3	1.96	0.47
2:M:164:PRO:HA	2:M:266:ARG:CZ	2.44	0.47
2:M:164:PRO:CA	2:M:266:ARG:HH12	2.23	0.47
9:C:9757:HOH:O	3:D:948:THR:HG21	2.13	0.47
3:N:1046:GLN:HG2	9:N:9308:HOH:O	2.13	0.47
1:A:193:ASP:OD2	2:C:938:LYS:HD2	2.14	0.47
3:N:396:VAL:HG22	3:N:447:VAL:HB	1.97	0.47
3:D:928:ALA:O	3:D:931:LEU:HB2	2.14	0.47
3:N:704:ARG:HG2	9:N:9228:HOH:O	2.13	0.47
3:N:809:PRO:O	3:N:812:ALA:HB3	2.15	0.47
1:A:88:ARG:HD2	1:A:123:MET:HE2	1.96	0.47
3:N:136:ASP:CG	3:N:137:PRO:HD3	2.35	0.47
1:B:206:THR:HG22	1:B:209:GLU:HG3	1.95	0.47
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.35	0.47
2:M:926:PHE:HE1	9:M:2113:HOH:O	1.97	0.47
4:E:82:GLU:HG2	4:E:83:ASP:H	1.80	0.47
3:D:79:GLU:HG2	3:D:80:VAL:N	2.29	0.47
3:N:969:ARG:HD3	9:N:9710:HOH:O	2.13	0.47
3:N:734:GLU:HB3	9:N:9236:HOH:O	2.14	0.47
1:L:133:GLU:HG3	1:L:134:GLU:H	1.80	0.47
1:B:105:GLY:HA3	9:B:9797:HOH:O	2.14	0.47
3:N:1086:LEU:HD22	9:N:9961:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:CE1	3:D:1352:ILE:HD13	2.50	0.47
3:D:1210:SER:HA	9:D:2674:HOH:O	2.13	0.47
5:P:402:ASN:O	5:P:406:ARG:HD2	2.15	0.47
3:N:98:PRO:HG3	3:N:515:GLU:CB	2.37	0.47
2:M:939:ARG:HD2	9:M:9308:HOH:O	2.14	0.47
3:N:123:LEU:HD11	3:N:152:LEU:CD2	2.45	0.47
3:D:1487:VAL:HG12	3:D:1488:ASP:H	1.78	0.47
2:M:91:GLN:HA	2:M:119:PRO:HA	1.95	0.47
3:N:463:GLN:HB3	9:N:9580:HOH:O	2.14	0.47
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.49	0.47
2:M:403:SER:C	2:M:407:LYS:HE2	2.35	0.47
3:N:836:VAL:HG12	9:N:9618:HOH:O	2.14	0.47
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.97	0.47
5:P:161:GLN:HA	5:P:164:LYS:HD2	1.96	0.47
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.96	0.47
2:C:507:ARG:HG2	2:C:508:ILE:O	2.14	0.47
2:M:910:LYS:HB2	9:M:2099:HOH:O	2.14	0.47
2:C:728:HIS:C	2:C:729:LEU:HD22	2.35	0.47
1:A:228:PRO:HG3	9:A:9640:HOH:O	2.14	0.47
3:N:1161:GLU:HG2	3:N:1164:ARG:HB2	1.95	0.47
3:N:1396:GLU:HA	3:N:1399:ASP:OD2	2.14	0.47
2:M:444:PRO:HG2	2:M:452:ILE:CD1	2.45	0.47
3:N:1274:ILE:HB	3:N:1322:GLY:HA2	1.97	0.47
2:M:298:PHE:HB2	9:M:2564:HOH:O	2.13	0.47
4:O:30:LEU:O	4:O:35:PHE:HA	2.15	0.47
1:A:108:GLU:O	1:A:110:LYS:HG3	2.15	0.47
3:D:1353:GLN:O	3:D:1357:ARG:HD2	2.14	0.47
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	2.29	0.47
2:M:344:PHE:O	2:M:348:LEU:HD13	2.14	0.47
3:N:62:LYS:HE2	9:N:2079:HOH:O	2.15	0.47
5:P:405:LEU:HD23	9:P:3207:HOH:O	2.13	0.47
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.96	0.47
2:C:988:VAL:N	9:C:9757:HOH:O	2.46	0.47
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.97	0.47
3:D:523:ASP:O	3:D:526:PRO:HG3	2.14	0.47
3:D:393:ILE:H	3:D:393:ILE:HG13	1.53	0.47
2:M:129:ILE:HG12	2:M:134:ARG:HD2	1.95	0.47
2:C:73:LEU:N	2:C:73:LEU:HD12	2.29	0.47
2:C:73:LEU:HD11	2:C:94:LEU:HD13	1.96	0.47
1:K:108:GLU:O	1:K:110:LYS:HG3	2.14	0.47
1:B:109:VAL:HG23	1:B:132:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:ALA:O	2:C:256:TYR:HB2	2.15	0.47
2:M:66:LEU:CD1	2:M:98:LEU:HD22	2.45	0.47
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.18	0.47
4:O:54:LEU:HG	4:O:58:PRO:CG	2.45	0.47
1:A:74:ASP:O	1:A:78:ILE:HG13	2.15	0.47
5:P:416:ARG:HH11	5:P:419:ARG:HB2	1.80	0.47
5:F:335:ASP:HB2	9:F:9582:HOH:O	2.15	0.47
2:C:953:VAL:HB	2:C:962:GLN:CG	2.45	0.47
2:M:586:ARG:HB3	2:M:586:ARG:HH11	1.79	0.47
3:N:785:ILE:HD12	3:N:785:ILE:H	1.80	0.47
3:N:1310:ARG:O	3:N:1327:ARG:HB2	2.15	0.47
3:N:1189:ARG:HA	3:N:1189:ARG:HH11	1.80	0.47
3:D:838:ARG:HH12	3:D:863:VAL:CG1	2.27	0.47
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.49	0.47
3:D:613:ARG:HA	9:D:9688:HOH:O	2.15	0.47
2:C:536:PRO:HD2	2:C:537:LYS:HZ1	1.80	0.47
5:P:182:ALA:O	5:P:185:GLN:HB2	2.14	0.47
3:D:804:LEU:HD21	3:D:829:VAL:CG2	2.42	0.47
3:N:400:VAL:HA	3:N:442:ASN:O	2.14	0.47
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.95	0.47
1:B:41:ARG:HG3	1:B:177:VAL:HB	1.95	0.47
1:A:176:ARG:HA	9:A:9583:HOH:O	2.14	0.47
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.15	0.47
2:C:250:ARG:HH21	2:C:254:VAL:HB	1.79	0.47
3:D:646:LYS:HG3	3:D:647:ARG:N	2.29	0.47
1:K:48:ILE:HA	1:K:49:PRO:HD3	1.75	0.47
2:C:403:SER:C	2:C:407:LYS:HD3	2.34	0.47
5:P:288:TYR:HA	5:P:291:ILE:CG2	2.45	0.47
3:N:998:GLU:O	3:N:1002:LYS:HG3	2.13	0.47
2:C:408:ARG:HD2	2:C:542:VAL:CG2	2.44	0.47
3:N:93:ILE:HG12	3:N:548:ILE:HD11	1.97	0.47
3:D:893:GLU:O	3:D:896:ALA:HB3	2.15	0.47
2:M:261:ILE:HG22	2:M:262:ALA:N	2.29	0.47
3:D:60:CYS:SG	3:D:62:LYS:HG2	2.54	0.47
3:N:210:ARG:HB3	9:N:9661:HOH:O	2.15	0.47
5:P:396:ARG:HD2	9:P:6184:HOH:O	2.14	0.47
2:C:1005:MET:SD	3:D:648:MET:HB2	2.55	0.47
2:C:603:VAL:O	2:C:646:GLY:HA2	2.15	0.47
5:F:209:PHE:O	5:F:213:ILE:HG13	2.14	0.47
2:C:346:VAL:O	2:C:350:ARG:HG3	2.15	0.47
2:M:799:ILE:HD13	2:M:799:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1182:GLU:HG3	9:N:9246:HOH:O	2.14	0.47
2:C:1072:LYS:HD3	9:C:9670:HOH:O	2.14	0.47
5:P:257:THR:CB	5:P:314:PRO:HG3	2.45	0.47
3:D:1084:THR:HG23	9:D:2894:HOH:O	2.13	0.47
2:C:524:VAL:HG22	2:C:528:GLU:HB2	1.96	0.47
3:D:1271:LYS:HD2	3:D:1334:GLN:OE1	2.14	0.47
5:F:226:LYS:HB2	9:F:9706:HOH:O	2.15	0.47
3:N:840:LYS:HA	9:N:9609:HOH:O	2.14	0.47
3:N:754:PHE:O	3:N:757:ALA:HB3	2.15	0.47
3:N:1406:ARG:HG2	3:N:1406:ARG:O	2.15	0.47
2:M:432:ARG:HD3	2:M:432:ARG:H	1.80	0.47
3:D:579:ASP:HB2	9:D:9699:HOH:O	2.14	0.47
2:C:458:TYR:O	2:C:460:ARG:HD2	2.14	0.47
3:D:493:ARG:HD3	3:D:1390:LEU:HD21	1.97	0.47
2:C:877:PRO:HD3	3:D:949:ILE:CD1	2.44	0.47
3:N:445:ARG:HG2	3:N:445:ARG:HH11	1.80	0.47
2:M:47:ALA:HA	2:M:50:GLU:OE2	2.14	0.47
3:D:50:PHE:O	3:D:86:ARG:HA	2.14	0.47
3:N:17:LYS:HG2	3:N:21:TRP:CE2	2.50	0.47
5:F:276:ARG:HB3	9:F:9760:HOH:O	2.15	0.47
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.44	0.47
4:E:48:MET:CB	4:E:54:LEU:HB2	2.39	0.47
3:N:704:ARG:HD3	9:N:9228:HOH:O	2.14	0.47
5:F:369:LEU:O	5:F:373:LYS:HB2	2.14	0.47
2:M:257:VAL:C	2:M:259:GLY:H	2.18	0.47
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.97	0.47
3:D:959:GLU:HB2	3:D:963:TYR:CE1	2.49	0.47
3:D:447:VAL:HG23	9:D:9599:HOH:O	2.14	0.47
3:D:1404:ASN:CG	3:D:1408:ILE:HD12	2.35	0.47
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.96	0.47
1:K:45:LEU:HD21	1:K:177:VAL:HG23	1.97	0.47
3:D:1448:THR:O	3:D:1451:ALA:HB3	2.15	0.47
5:F:406:ARG:HA	5:F:409:LYS:CD	2.45	0.47
1:A:106:PRO:HG3	9:A:9569:HOH:O	2.15	0.47
3:D:644:LEU:HD12	3:D:644:LEU:O	2.15	0.47
2:M:1074:GLU:HG3	9:M:2120:HOH:O	2.13	0.47
2:C:651:LYS:HE3	9:C:2035:HOH:O	2.15	0.47
1:B:192:LEU:HG	9:B:9584:HOH:O	2.15	0.47
2:C:916:GLU:O	2:C:919:ALA:HB3	2.15	0.47
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.96	0.47
2:M:283:ILE:HG12	9:M:9557:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:9:LEU:HB3	4:O:19:LEU:HD21	1.96	0.47
2:C:749:VAL:HA	9:C:9864:HOH:O	2.15	0.47
5:P:284:ARG:HB3	9:P:4605:HOH:O	2.15	0.47
5:F:245:GLN:HA	9:F:9828:HOH:O	2.13	0.47
2:C:1039:ALA:CB	3:D:713:ILE:HD12	2.45	0.47
2:C:100:LEU:CD2	2:C:368:THR:HA	2.44	0.47
2:C:1085:PHE:O	2:C:1088:LEU:HB3	2.15	0.47
3:D:475:LYS:O	3:D:478:LEU:HB2	2.15	0.47
2:C:165:LEU:HD12	2:C:166:PRO:C	2.36	0.47
5:F:397:ILE:HG21	9:F:9936:HOH:O	2.14	0.47
2:C:1016:ILE:HD13	2:C:1016:ILE:N	2.29	0.47
3:N:1148:VAL:O	3:N:1189:ARG:HG2	2.15	0.47
3:D:601:ARG:HH22	3:D:613:ARG:HE	1.63	0.47
9:M:9896:HOH:O	5:P:373:LYS:HB3	2.14	0.47
5:P:191:ASN:HA	9:P:1478:HOH:O	2.15	0.47
3:N:1033:GLN:HA	9:N:2161:HOH:O	2.14	0.47
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	1.98	0.47
3:N:607:LEU:HA	9:N:2546:HOH:O	2.15	0.47
3:N:974:ILE:HG12	3:N:991:GLN:HE21	1.79	0.47
2:M:346:VAL:HG12	2:M:350:ARG:NE	2.29	0.47
2:M:342:ASP:O	2:M:346:VAL:HG23	2.15	0.47
1:K:152:PRO:HD2	1:K:155:LYS:HB2	1.97	0.47
2:M:701:THR:HG22	2:M:832:LYS:HA	1.97	0.47
2:M:782:ALA:HB1	9:M:9603:HOH:O	2.14	0.47
3:D:1217:ILE:HD13	3:D:1480:PHE:CE2	2.49	0.47
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.15	0.47
3:D:1045:MET:HA	9:D:2022:HOH:O	2.14	0.47
2:M:165:LEU:HD12	2:M:166:PRO:C	2.35	0.47
3:D:445:ARG:HG2	3:D:445:ARG:NH1	2.30	0.47
2:M:1083:GLU:O	2:M:1087:VAL:HG23	2.15	0.47
2:C:253:ALA:HB3	9:C:2420:HOH:O	2.14	0.47
2:M:310:LEU:HD11	9:M:2059:HOH:O	2.15	0.47
2:M:676:ILE:CG2	2:M:988:VAL:HG13	2.44	0.47
2:M:871:LEU:HD12	2:M:872:ASN:O	2.14	0.47
1:L:90:LEU:HD21	9:L:3389:HOH:O	2.15	0.47
3:D:54:LYS:HA	5:F:337:HIS:HE1	1.80	0.47
1:A:6:LEU:C	1:A:8:ALA:H	2.18	0.47
3:D:676:MET:HE1	3:D:684:LYS:H	1.80	0.47
1:K:184:THR:HG22	1:K:192:LEU:O	2.15	0.47
3:D:1339:LYS:HG2	3:D:1343:ALA:HB2	1.97	0.47
2:M:152:PRO:HD2	9:M:9283:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1020:LEU:HA	3:N:1023:MET:HE2	1.97	0.47
3:N:1134:LEU:HB2	9:N:2308:HOH:O	2.15	0.47
2:C:913:GLU:O	2:C:916:GLU:HB3	2.15	0.47
3:D:1194:CYS:SG	3:D:1200:VAL:HA	2.55	0.47
5:P:99:GLU:OE1	5:P:235:PHE:HB3	2.15	0.47
1:K:138:LEU:HB2	9:K:8021:HOH:O	2.15	0.47
5:F:142:ARG:HA	9:F:9681:HOH:O	2.15	0.47
2:M:165:LEU:HD21	2:M:334:ARG:HH21	1.79	0.46
3:N:1052:THR:HG22	9:N:9337:HOH:O	2.15	0.46
2:C:89:THR:HG22	2:C:91:GLN:HG3	1.97	0.46
5:F:166:LEU:HD13	5:F:170:HIS:CB	2.44	0.46
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.96	0.46
2:M:600:ASP:HA	9:M:2442:HOH:O	2.14	0.46
3:N:1219:GLU:HG3	4:O:17:TYR:OH	2.15	0.46
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.45	0.46
3:N:1188:VAL:HG22	3:N:1189:ARG:O	2.15	0.46
3:D:865:THR:HG22	9:D:9766:HOH:O	2.14	0.46
4:O:39:VAL:HG12	9:O:1697:HOH:O	2.14	0.46
5:P:106:VAL:HA	9:P:1566:HOH:O	2.15	0.46
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.98	0.46
2:C:184:MET:HE1	2:C:186:VAL:N	2.30	0.46
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.80	0.46
3:N:686:GLU:HG2	9:N:2678:HOH:O	2.14	0.46
1:L:108:GLU:O	1:L:110:LYS:HG3	2.15	0.46
3:N:566:ILE:CD1	5:P:217:ASN:HD22	2.28	0.46
2:C:41:ASN:H	2:C:41:ASN:ND2	2.12	0.46
2:M:485:TYR:HD2	9:M:9411:HOH:O	1.97	0.46
3:D:992:ILE:HA	9:D:2129:HOH:O	2.14	0.46
5:P:359:SER:HA	9:P:1489:HOH:O	2.15	0.46
2:C:942:GLU:HG3	9:C:9752:HOH:O	2.14	0.46
1:K:54:THR:HG21	1:K:145:ASP:OD1	2.15	0.46
3:D:702:LEU:HD13	3:D:716:PHE:HD1	1.81	0.46
2:C:369:PRO:HG2	9:C:2433:HOH:O	2.15	0.46
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.15	0.46
4:E:76:GLY:N	4:E:79:LEU:HD22	2.29	0.46
2:M:151:ASP:HB2	2:M:157:ARG:O	2.15	0.46
3:D:458:ALA:HB2	9:D:2106:HOH:O	2.15	0.46
5:F:287:THR:CG2	5:F:289:GLU:HB2	2.41	0.46
2:C:517:ARG:HB2	9:C:9578:HOH:O	2.15	0.46
5:F:365:GLU:O	5:F:369:LEU:HD12	2.15	0.46
1:A:50:GLY:N	9:A:9574:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:711:LEU:C	3:N:713:ILE:H	2.19	0.46
4:O:39:VAL:HA	9:O:1697:HOH:O	2.15	0.46
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.98	0.46
5:P:166:LEU:HD22	5:P:170:HIS:HB2	1.98	0.46
3:D:1165:TYR:HB2	9:D:9690:HOH:O	2.15	0.46
5:P:315:VAL:HG12	5:P:316:SER:H	1.80	0.46
9:C:9869:HOH:O	3:D:1068:LEU:HD13	2.15	0.46
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.51	0.46
2:C:899:GLN:OE1	2:C:901:TYR:HE2	1.98	0.46
3:D:754:PHE:CE2	3:D:1476:THR:HG21	2.49	0.46
3:D:207:PHE:HB3	3:D:395:VAL:HG21	1.97	0.46
2:M:19:THR:HG22	2:M:23:VAL:HG23	1.97	0.46
3:N:36:THR:O	3:N:38:LYS:N	2.48	0.46
2:C:678:PRO:HG3	2:C:873:PRO:HD2	1.96	0.46
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.46	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HD12	1.97	0.46
3:D:542:ASP:HA	3:D:545:ARG:HE	1.80	0.46
2:C:217:LEU:HD23	9:C:9668:HOH:O	2.15	0.46
5:P:264:MET:O	5:P:268:ILE:HG13	2.16	0.46
1:A:191:ASP:O	1:A:192:LEU:HD23	2.16	0.46
2:M:278:GLU:HG3	2:M:283:ILE:O	2.16	0.46
2:C:2:GLU:HG2	9:C:2528:HOH:O	2.16	0.46
5:P:192:LEU:HD22	9:P:4506:HOH:O	2.15	0.46
2:C:591:SER:HB2	9:C:9610:HOH:O	2.15	0.46
2:C:35:PRO:HD2	2:C:38:LYS:CE	2.46	0.46
3:N:168:THR:OG1	3:N:393:ILE:HD12	2.15	0.46
2:M:773:LEU:HD11	5:P:405:LEU:HD13	1.97	0.46
2:M:950:LEU:HD12	2:M:952:LEU:HD21	1.97	0.46
2:M:313:LEU:C	2:M:315:ALA:H	2.17	0.46
3:D:172:PRO:HB3	3:D:178:LEU:HB3	1.98	0.46
3:N:433:GLY:HA3	3:N:450:TYR:HA	1.96	0.46
2:C:91:GLN:HA	2:C:119:PRO:HA	1.96	0.46
2:C:246:ASP:HB2	9:C:2442:HOH:O	2.15	0.46
3:N:829:VAL:HG22	9:N:9736:HOH:O	2.15	0.46
2:C:737:LEU:HD11	2:C:754:ILE:HG21	1.95	0.46
2:C:1102:LEU:N	3:D:7:LYS:O	2.48	0.46
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.96	0.46
2:C:861:LEU:CD2	2:C:863:ASP:H	2.28	0.46
3:D:206:ARG:HA	3:D:206:ARG:HH11	1.80	0.46
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.15	0.46
5:P:109:GLY:HA3	9:P:1566:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:725:ASP:O	2:M:727:PRO:HD3	2.15	0.46
1:K:162:ILE:HG13	1:K:163:ASN:ND2	2.30	0.46
2:C:230:ARG:HB2	2:C:233:GLU:HB3	1.97	0.46
3:N:1031:ASN:OD1	3:N:1033:GLN:HB2	2.15	0.46
1:B:115:LEU:O	1:B:115:LEU:HD12	2.14	0.46
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.96	0.46
3:N:686:GLU:HG3	9:N:2781:HOH:O	2.14	0.46
1:K:29:GLU:HB3	9:K:4304:HOH:O	2.14	0.46
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.46
5:F:147:LEU:HD23	9:F:9698:HOH:O	2.15	0.46
5:P:351:SER:HB2	9:P:6220:HOH:O	2.15	0.46
2:C:657:ASP:OD1	2:C:661:SER:HB2	2.14	0.46
2:C:933:GLY:HA2	9:C:2021:HOH:O	2.16	0.46
1:B:213:GLN:O	1:B:217:ILE:HG13	2.15	0.46
3:N:408:GLU:HG2	9:N:9546:HOH:O	2.15	0.46
3:N:1340:GLY:O	3:N:1344:VAL:HG23	2.15	0.46
2:C:422:ARG:HD3	9:C:2680:HOH:O	2.16	0.46
3:D:13:ALA:O	3:D:511:TRP:HB3	2.15	0.46
2:M:546:LEU:HA	2:M:581:THR:OG1	2.15	0.46
3:D:1209:LEU:HD13	3:D:1219:GLU:OE2	2.15	0.46
4:O:41:GLU:H	4:O:42:PRO:HD2	1.80	0.46
4:O:41:GLU:CA	4:O:45:ARG:HG3	2.45	0.46
4:O:40:LEU:CG	4:O:67:GLU:HG2	2.45	0.46
3:D:919:PHE:HA	3:D:927:THR:OG1	2.16	0.46
1:A:217:ILE:HB	9:A:9598:HOH:O	2.15	0.46
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.98	0.46
3:N:842:VAL:HG23	9:N:9393:HOH:O	2.14	0.46
1:L:75:VAL:O	1:L:79:ILE:HG23	2.15	0.46
3:N:806:PHE:HE1	3:N:813:LEU:HB3	1.80	0.46
3:N:827:ILE:O	3:N:837:GLY:HA3	2.15	0.46
3:D:1379:VAL:O	3:D:1392:GLY:HA2	2.16	0.46
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.46	0.46
1:A:197:LEU:HD23	1:A:197:LEU:N	2.27	0.46
2:M:480:THR:HG22	2:M:482:GLU:N	2.30	0.46
2:M:560:MET:O	2:M:564:MET:HB2	2.15	0.46
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.45	0.46
3:N:1478:SER:C	3:N:1480:PHE:H	2.17	0.46
5:P:231:ARG:HA	9:P:2972:HOH:O	2.15	0.46
2:C:922:PHE:HD2	9:C:2177:HOH:O	1.99	0.46
2:C:313:LEU:C	2:C:315:ALA:H	2.18	0.46
2:C:1059:ASP:N	9:C:9720:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1351:GLU:O	3:D:1354:LYS:HB2	2.16	0.46
3:N:65:ARG:HG2	5:P:375:LEU:HA	1.98	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.20	0.46
3:D:523:ASP:N	3:D:523:ASP:OD1	2.47	0.46
2:M:841:ASN:ND2	2:M:845:ASN:N	2.64	0.46
3:D:534:ARG:HG3	9:D:2518:HOH:O	2.15	0.46
2:C:129:ILE:N	2:C:129:ILE:HD12	2.31	0.46
5:P:416:ARG:HA	9:P:4146:HOH:O	2.15	0.46
3:N:1192:LEU:HD22	3:N:1345:GLU:OE2	2.14	0.46
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.45	0.46
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.97	0.46
2:M:19:THR:HG22	2:M:19:THR:O	2.15	0.46
1:K:184:THR:O	1:K:192:LEU:HD12	2.15	0.46
3:D:431:VAL:HG12	9:D:2014:HOH:O	2.15	0.46
3:N:772:PRO:HG3	9:N:9333:HOH:O	2.15	0.46
2:M:564:MET:HG2	2:M:840:ALA:CB	2.46	0.46
3:N:1044:LEU:CD2	3:N:1056:PRO:HG3	2.46	0.46
2:C:524:VAL:HG22	2:C:525:SER:H	1.81	0.46
3:D:446:VAL:HG11	9:D:9698:HOH:O	2.15	0.46
2:M:504:GLU:HA	9:M:9395:HOH:O	2.16	0.46
2:C:498:GLN:HG3	9:C:9570:HOH:O	2.16	0.46
4:O:86:GLN:O	4:O:90:GLU:HG3	2.15	0.46
2:M:544:THR:HA	2:M:562:SER:OG	2.15	0.46
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.80	0.46
5:P:367:MET:HA	5:P:370:LYS:HG2	1.98	0.46
2:M:145:GLY:H	2:M:163:ILE:CG2	2.28	0.46
2:M:288:ARG:NH1	2:M:288:ARG:HG3	2.26	0.46
2:M:578:VAL:HG21	2:M:991:GLN:O	2.16	0.46
2:C:89:THR:O	2:C:91:GLN:HG3	2.14	0.46
3:N:414:ARG:HA	9:N:9486:HOH:O	2.16	0.46
3:D:704:ARG:CD	3:D:705:ALA:H	2.25	0.46
2:M:207:LEU:O	2:M:211:LEU:HB3	2.16	0.46
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.80	0.46
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.46
2:C:358:ARG:HB3	2:C:371:LYS:O	2.16	0.46
2:C:751:PRO:HB2	3:D:680:GLN:CG	2.44	0.46
3:N:1442:ASN:HD22	3:N:1443:THR:N	2.13	0.46
5:P:94:LEU:HB3	5:P:98:GLU:H	1.81	0.46
3:D:687:VAL:O	3:D:690:ALA:HB3	2.15	0.46
2:C:250:ARG:HD2	9:C:9629:HOH:O	2.15	0.46
2:C:187:ASN:HB3	9:C:9640:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:LEU:O	1:K:115:LEU:HD12	2.15	0.46
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.30	0.46
3:D:550:ARG:HG3	3:D:550:ARG:NH1	2.30	0.46
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.97	0.46
1:L:134:GLU:HG2	9:L:6529:HOH:O	2.16	0.46
4:O:13:VAL:HG11	4:O:19:LEU:HB2	1.98	0.46
3:D:1051:GLU:HB3	9:D:2777:HOH:O	2.15	0.46
5:P:349:LEU:HD23	9:P:2092:HOH:O	2.16	0.46
3:N:1385:GLY:HA2	3:N:1413:THR:HG21	1.97	0.46
2:M:630:ARG:HH11	2:M:630:ARG:HG3	1.80	0.46
4:E:39:VAL:HA	9:E:9571:HOH:O	2.14	0.46
3:N:1158:VAL:HG12	3:N:1159:ARG:N	2.31	0.46
9:C:9607:HOH:O	3:D:18:ILE:HD11	2.14	0.46
3:D:1354:LYS:HD3	9:D:2684:HOH:O	2.15	0.46
2:C:671:ASN:HD22	2:C:993:PHE:HD2	1.64	0.46
3:D:711:LEU:C	3:D:713:ILE:H	2.18	0.46
3:D:1384:PRO:HG3	3:D:1389:LEU:N	2.31	0.46
3:N:127:LEU:HD12	3:N:128:TYR:N	2.30	0.46
2:M:265:ARG:HD2	9:M:2426:HOH:O	2.15	0.46
5:F:267:THR:HA	5:F:270:LYS:HZ2	1.80	0.46
2:C:141:HIS:HE1	2:C:332:ARG:HE	1.62	0.46
2:C:464:LEU:HB3	9:C:2642:HOH:O	2.16	0.46
2:M:724:ARG:HB2	2:M:741:GLY:N	2.31	0.46
3:N:861:GLN:HB2	9:N:9290:HOH:O	2.14	0.46
2:M:586:ARG:HH12	2:M:590:ASP:CG	2.19	0.46
1:L:83:LYS:HG2	9:L:4413:HOH:O	2.15	0.46
3:N:702:LEU:O	3:N:713:ILE:HA	2.15	0.46
2:C:148:PHE:HE1	2:C:281:LEU:HD22	1.80	0.46
2:M:281:LEU:HB2	2:M:309:TYR:CD1	2.51	0.46
3:D:32:ILE:HG13	3:D:45:PHE:HD2	1.80	0.46
1:K:41:ARG:NH1	1:K:177:VAL:HB	2.29	0.46
4:O:94:PRO:HA	9:O:9005:HOH:O	2.15	0.46
2:M:1104:GLU:O	3:N:7:LYS:HE2	2.15	0.46
3:D:166:GLN:HB3	3:D:395:VAL:CG2	2.46	0.46
2:M:1036:GLU:HG3	3:N:707:THR:OG1	2.15	0.46
2:M:564:MET:CE	2:M:846:LYS:HE2	2.45	0.46
2:M:770:GLU:HA	2:M:770:GLU:OE2	2.15	0.46
3:N:649:ALA:HB3	3:N:691:LEU:HD21	1.97	0.46
3:N:770:LEU:HD23	3:N:777:PRO:HA	1.98	0.46
9:D:9992:HOH:O	5:F:168:LYS:HG2	2.15	0.46
3:D:1294:VAL:HG13	9:D:2676:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1236:LEU:HA	3:N:1359:GLN:OE1	2.16	0.46
3:D:202:VAL:O	3:D:204:LEU:HG	2.15	0.46
2:C:1059:ASP:OD1	2:C:1080:SER:HB2	2.16	0.46
3:N:65:ARG:HG2	5:P:374:GLY:O	2.15	0.46
2:C:405:ARG:HH22	2:C:409:ARG:HH21	1.63	0.46
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.17	0.46
1:L:185:ARG:HH12	3:N:692:GLU:HG3	1.79	0.46
3:D:1026:SER:HB2	9:D:9566:HOH:O	2.15	0.46
2:M:1083:GLU:HG2	9:M:9233:HOH:O	2.16	0.46
2:C:870:ILE:HD12	2:C:870:ILE:N	2.31	0.46
2:M:585:GLU:O	2:M:588:VAL:HG22	2.16	0.46
2:C:1102:LEU:CD1	3:D:9:ARG:HG2	2.45	0.46
2:C:774:LEU:HB2	9:C:2198:HOH:O	2.15	0.46
3:D:1144:LEU:HD11	3:D:1186:VAL:HG21	1.96	0.46
4:E:51:LEU:HD22	9:E:9663:HOH:O	2.16	0.46
2:C:723:THR:HA	9:C:9700:HOH:O	2.15	0.46
3:N:756:GLN:O	3:N:760:ARG:HG2	2.15	0.46
5:P:93:LEU:CD2	5:P:98:GLU:HB3	2.46	0.46
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.51	0.46
1:L:182:GLU:O	1:L:194:LYS:HB3	2.16	0.46
2:M:713:ARG:HH11	2:M:713:ARG:HG2	1.81	0.46
3:D:438:ASP:OD2	3:D:440:VAL:HB	2.16	0.46
2:C:756:VAL:CG2	2:C:823:VAL:HG11	2.45	0.46
3:N:687:VAL:O	3:N:690:ALA:HB3	2.15	0.46
2:C:455:LEU:HD22	2:C:459:ALA:CB	2.46	0.46
3:D:814:ALA:O	3:D:818:ARG:HG3	2.16	0.46
2:C:626:ARG:NH1	2:C:637:LEU:HD12	2.30	0.46
2:M:749:VAL:O	2:M:749:VAL:HG23	2.15	0.46
1:B:95:GLN:HB3	9:B:9815:HOH:O	2.15	0.46
5:P:87:GLU:O	5:P:91:VAL:HG23	2.16	0.46
2:M:22:GLN:O	2:M:121:MET:HE1	2.16	0.46
3:N:187:LYS:HA	9:N:9419:HOH:O	2.16	0.46
3:N:186:VAL:HG13	3:N:187:LYS:N	2.31	0.46
3:N:1076:GLY:HA2	3:N:1079:LYS:HG2	1.98	0.46
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.98	0.46
3:D:1376:MET:HG2	3:D:1421:LEU:HA	1.97	0.46
2:M:404:LEU:HA	2:M:407:LYS:HE2	1.98	0.46
3:N:395:VAL:O	3:N:395:VAL:HG12	2.16	0.46
2:C:1000:MET:HB2	2:C:1002:GLU:HG2	1.97	0.46
3:D:104:PHE:HE2	3:D:1448:THR:HA	1.81	0.46
1:B:201:THR:HG22	1:B:203:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:220:LEU:O	5:P:224:VAL:HG23	2.16	0.46
2:C:408:ARG:HD2	2:C:542:VAL:HG21	1.98	0.46
2:M:946:ARG:HB2	9:M:9918:HOH:O	2.16	0.46
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.45	0.46
5:P:125:ASP:HB2	9:P:8230:HOH:O	2.16	0.46
1:K:75:VAL:O	1:K:79:ILE:HG23	2.16	0.46
2:C:597:ALA:O	2:C:652:GLY:N	2.47	0.46
3:N:657:LEU:O	3:N:661:MET:HG2	2.16	0.46
3:N:27:GLU:N	9:N:9304:HOH:O	2.49	0.46
3:D:1293:PHE:HB3	9:D:9737:HOH:O	2.15	0.46
2:M:613:VAL:HB	9:M:9426:HOH:O	2.14	0.46
3:D:493:ARG:O	3:D:497:GLU:HG2	2.16	0.46
2:C:66:LEU:HD11	2:C:98:LEU:HD22	1.98	0.46
3:D:154:THR:HG22	3:D:155:ASP:H	1.81	0.46
2:M:839:LEU:HD11	2:M:849:VAL:HG22	1.98	0.46
1:A:209:GLU:O	1:A:213:GLN:HG3	2.16	0.46
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.46	0.46
3:N:525:ARG:N	3:N:526:PRO:HD3	2.31	0.46
1:K:70:GLY:HA2	1:K:133:GLU:CG	2.46	0.46
2:M:1056:LYS:HB3	3:N:624:ASP:H	1.80	0.46
2:C:724:ARG:HB2	2:C:740:GLU:CA	2.42	0.46
5:P:394:ARG:HB3	9:P:6528:HOH:O	2.16	0.46
2:C:887:GLU:OE1	2:C:992:MET:HA	2.15	0.46
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.15	0.46
3:N:1498:ALA:HB2	9:N:9438:HOH:O	2.16	0.46
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.97	0.46
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.28	0.46
2:C:133:ASP:HB2	2:C:632:ASN:ND2	2.27	0.46
1:B:19:GLU:HG3	9:B:9589:HOH:O	2.15	0.46
5:F:220:LEU:O	5:F:223:ALA:HB3	2.16	0.46
3:N:138:LYS:HD3	9:N:9902:HOH:O	2.16	0.46
2:C:768:THR:HG22	2:C:771:GLU:H	1.81	0.46
2:C:808:ARG:HD3	9:C:2330:HOH:O	2.15	0.46
3:N:38:LYS:NZ	3:N:59:ALA:HB1	2.30	0.46
3:N:50:PHE:O	3:N:86:ARG:HA	2.15	0.46
3:D:508:ARG:HA	3:D:509:PRO:HD2	1.71	0.46
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.97	0.46
3:D:649:ALA:HB3	3:D:691:LEU:HD21	1.97	0.46
2:C:569:VAL:HG12	2:C:996:LYS:O	2.16	0.46
2:M:115:LEU:HD12	2:M:115:LEU:O	2.16	0.46
3:D:465:LEU:HD22	3:D:510:GLU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1097:LYS:HD2	9:D:9821:HOH:O	2.16	0.45
3:D:1375:MET:SD	3:D:1423:GLY:HA2	2.55	0.45
3:D:90:MET:HE3	3:D:520:LEU:HA	1.97	0.45
3:D:521:PRO:C	3:D:525:ARG:HH11	2.20	0.45
2:C:157:ARG:HD2	2:C:314:THR:CG2	2.39	0.45
2:C:1097:LEU:CD2	2:C:1097:LEU:H	2.20	0.45
2:M:1060:ILE:HG12	2:M:1063:ARG:NH2	2.30	0.45
3:D:1122:LEU:HD12	3:D:1122:LEU:N	2.30	0.45
5:F:371:LEU:CD2	5:F:375:LEU:HD22	2.45	0.45
1:B:50:GLY:HA3	1:B:171:PHE:O	2.16	0.45
2:C:721:ARG:HA	9:C:2273:HOH:O	2.16	0.45
2:C:6:PHE:HA	2:C:8:ARG:HH21	1.80	0.45
3:N:651:GLU:HG2	9:N:2423:HOH:O	2.16	0.45
3:D:1283:ILE:HG22	3:D:1284:GLU:H	1.81	0.45
2:C:815:LEU:HD21	2:C:819:VAL:O	2.16	0.45
2:C:1:MET:SD	2:C:900:ARG:HD3	2.56	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.97	0.45
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.97	0.45
2:M:818:GLY:HA3	9:M:2517:HOH:O	2.16	0.45
1:B:14:ARG:HA	9:B:9663:HOH:O	2.15	0.45
5:P:289:GLU:O	5:P:293:GLU:HG3	2.17	0.45
2:C:1058:ASP:CG	2:C:1084:SER:H	2.19	0.45
3:N:445:ARG:H	3:N:445:ARG:HD2	1.79	0.45
2:C:945:ARG:HB3	9:C:2615:HOH:O	2.17	0.45
2:C:208:ALA:HB1	2:C:218:VAL:HG11	1.97	0.45
3:D:464:LEU:O	3:D:468:LEU:HG	2.16	0.45
5:F:309:LYS:HD3	9:F:9794:HOH:O	2.16	0.45
3:D:1146:GLY:CA	3:D:1207:TYR:HB2	2.39	0.45
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.98	0.45
3:N:928:ALA:O	3:N:931:LEU:HB2	2.15	0.45
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.42	0.45
2:C:17:PRO:O	2:C:20:GLU:HB3	2.17	0.45
2:C:24:GLU:HA	9:C:2056:HOH:O	2.15	0.45
5:F:173:TYR:HA	5:F:176:ILE:HD12	1.97	0.45
2:M:174:LEU:HB2	2:M:310:LEU:HD22	1.99	0.45
5:F:214:GLN:O	5:F:217:ASN:HB2	2.16	0.45
1:K:33:GLY:O	1:K:195:LEU:HD13	2.17	0.45
2:M:399:ASN:ND2	2:M:568:ALA:HB3	2.31	0.45
3:D:1121:PRO:C	3:D:1122:LEU:HD12	2.36	0.45
3:N:166:GLN:HE21	3:N:167:GLU:C	2.19	0.45
2:M:16:PRO:HB3	2:M:460:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HE3	1:A:5:LYS:HA	1.97	0.45
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.16	0.45
3:D:1188:VAL:HG22	3:D:1189:ARG:O	2.15	0.45
3:N:468:LEU:HD12	9:N:9350:HOH:O	2.16	0.45
5:P:266:GLU:HB2	5:P:270:LYS:HZ2	1.80	0.45
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.98	0.45
2:C:768:THR:HG23	9:C:2074:HOH:O	2.16	0.45
1:K:212:ASN:HD22	1:K:212:ASN:N	2.13	0.45
2:C:585:GLU:HG2	2:C:665:PHE:CD2	2.51	0.45
2:M:252:LYS:HE2	2:M:296:GLY:HA3	1.97	0.45
3:N:919:PHE:HA	3:N:927:THR:OG1	2.17	0.45
3:D:11:ALA:HB2	9:D:9902:HOH:O	2.14	0.45
3:D:125:GLN:HE22	3:D:587:ARG:HE	1.65	0.45
5:F:238:TYR:HB2	9:F:9643:HOH:O	2.16	0.45
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.99	0.45
3:D:148:GLU:HG2	9:D:9755:HOH:O	2.15	0.45
5:P:366:ALA:HB2	9:P:1329:HOH:O	2.15	0.45
3:D:84:ILE:HG13	3:D:85:VAL:N	2.31	0.45
3:D:178:LEU:HD11	9:D:2532:HOH:O	2.15	0.45
2:M:841:ASN:ND2	2:M:845:ASN:HB3	2.32	0.45
2:M:194:VAL:HG13	2:M:221:LEU:HD12	1.97	0.45
3:D:577:ALA:O	3:D:580:ALA:HB3	2.17	0.45
2:C:962:GLN:N	9:C:9884:HOH:O	2.49	0.45
2:M:545:ASN:HB2	9:M:9531:HOH:O	2.16	0.45
3:N:737:ASN:C	9:N:9228:HOH:O	2.54	0.45
2:M:605:LYS:HD2	9:M:9417:HOH:O	2.16	0.45
1:K:57:TYR:CE1	1:K:163:ASN:HB2	2.46	0.45
2:M:627:ARG:HD2	9:M:9479:HOH:O	2.17	0.45
2:C:21:ILE:HD12	2:C:21:ILE:N	2.30	0.45
1:L:143:ARG:HB2	9:L:7130:HOH:O	2.15	0.45
3:N:660:LYS:O	3:N:664:LYS:HG3	2.16	0.45
2:M:955:PRO:HG2	9:M:9748:HOH:O	2.15	0.45
2:M:424:GLY:O	2:M:428:ARG:HG3	2.17	0.45
3:N:182:GLY:HA2	9:N:9237:HOH:O	2.15	0.45
3:N:479:GLU:HB3	9:N:9264:HOH:O	2.15	0.45
5:F:356:LYS:HD3	9:F:9676:HOH:O	2.15	0.45
2:C:685:GLU:HB3	9:C:2345:HOH:O	2.15	0.45
3:N:154:THR:HG23	3:N:157:GLU:H	1.81	0.45
3:D:710:ARG:HG3	3:D:711:LEU:N	2.31	0.45
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.98	0.45
5:P:405:LEU:HG	9:P:3208:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:273:GLY:HA2	9:M:9612:HOH:O	2.17	0.45
2:M:42:VAL:HG12	2:M:43:GLY:N	2.26	0.45
9:M:9246:HOH:O	5:P:345:ALA:HA	2.15	0.45
1:K:197:LEU:N	9:K:1736:HOH:O	2.48	0.45
2:M:492:ASP:CA	2:M:518:LYS:HB3	2.43	0.45
2:C:136:ILE:HD11	9:C:9782:HOH:O	2.15	0.45
2:C:288:ARG:HH11	2:C:288:ARG:HA	1.82	0.45
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.79	0.45
4:O:70:THR:HA	9:O:2214:HOH:O	2.16	0.45
2:M:187:ASN:HB3	9:M:2286:HOH:O	2.16	0.45
1:A:90:LEU:HA	9:A:9720:HOH:O	2.17	0.45
3:D:660:LYS:O	3:D:663:GLU:HB2	2.16	0.45
2:C:794:PRO:HD2	9:C:9926:HOH:O	2.16	0.45
5:F:93:LEU:CD2	5:F:98:GLU:HB3	2.46	0.45
1:A:89:PHE:HB2	9:A:9614:HOH:O	2.15	0.45
2:M:367:LEU:HA	2:M:371:LYS:HB2	1.98	0.45
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.99	0.45
3:N:1283:ILE:HG22	3:N:1284:GLU:H	1.82	0.45
1:A:198:ARG:HB2	1:A:200:TRP:CZ3	2.52	0.45
2:M:59:LYS:HB3	9:M:9726:HOH:O	2.16	0.45
2:M:1076:VAL:HG22	3:N:752:SER:HB3	1.98	0.45
3:D:1168:MET:HA	3:D:1168:MET:HE3	1.97	0.45
2:C:707:ARG:HG3	2:C:826:TYR:CZ	2.51	0.45
4:O:82:GLU:HG3	9:O:2121:HOH:O	2.17	0.45
2:M:353:ARG:HA	9:M:9887:HOH:O	2.16	0.45
5:F:230:LYS:HA	9:F:9842:HOH:O	2.16	0.45
3:D:1103:HIS:HA	3:D:1223:ILE:CD1	2.45	0.45
3:D:1428:ALA:C	3:D:1430:SER:H	2.18	0.45
3:D:500:ARG:HA	9:D:2025:HOH:O	2.16	0.45
2:M:1085:PHE:CE2	3:N:1468:LEU:HG	2.51	0.45
3:N:116:LEU:O	3:N:118:LEU:N	2.49	0.45
5:P:133:ALA:HB1	9:P:2305:HOH:O	2.15	0.45
2:C:584:GLU:O	2:C:588:VAL:HG13	2.16	0.45
2:M:1030:GLN:O	3:N:622:ARG:HA	2.17	0.45
3:D:1493:LYS:HE2	9:D:9651:HOH:O	2.16	0.45
3:N:704:ARG:HH12	3:N:743:ASP:HB3	1.79	0.45
1:B:80:LEU:HD13	3:D:842:VAL:HG12	1.98	0.45
3:N:701:LEU:C	3:N:702:LEU:HD12	2.37	0.45
2:M:183:SER:HA	2:M:190:LYS:HB2	1.99	0.45
2:M:727:PRO:HG3	2:M:783:ARG:CZ	2.47	0.45
2:M:16:PRO:O	2:M:18:LEU:HD12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:684:LYS:O	3:D:687:VAL:HG23	2.17	0.45
1:K:156:HIS:CD2	1:K:158:ILE:HG12	2.52	0.45
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.52	0.45
5:P:315:VAL:HG12	5:P:316:SER:N	2.31	0.45
3:D:1033:GLN:O	3:D:1036:ARG:HB3	2.16	0.45
3:D:1356:TYR:HD2	3:D:1361:VAL:HG11	1.82	0.45
2:M:502:PRO:HA	9:M:2305:HOH:O	2.16	0.45
3:N:1176:LYS:O	3:N:1179:GLU:HB2	2.17	0.45
2:C:204:GLN:HB2	9:C:2456:HOH:O	2.17	0.45
3:N:1114:THR:HG22	3:N:1195:GLN:HB2	1.97	0.45
3:N:543:LEU:O	3:N:546:ARG:HB2	2.16	0.45
3:N:577:ALA:O	3:N:580:ALA:HB3	2.17	0.45
3:D:1343:ALA:HA	9:D:2807:HOH:O	2.15	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.99	0.45
2:M:292:ARG:CZ	2:M:299:LYS:HD3	2.47	0.45
5:P:292:ALA:O	5:P:299:TRP:HB2	2.15	0.45
3:N:1299:PHE:HB2	9:N:2802:HOH:O	2.16	0.45
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.17	0.45
3:N:1409:ALA:HB2	9:N:9520:HOH:O	2.16	0.45
4:O:77:GLU:HB2	9:O:2132:HOH:O	2.15	0.45
1:B:226:SER:O	1:B:228:PRO:HD3	2.16	0.45
3:D:4:GLU:HG3	9:D:2516:HOH:O	2.15	0.45
3:N:1054:GLU:HB2	9:N:9784:HOH:O	2.17	0.45
2:C:820:ARG:HA	9:C:2072:HOH:O	2.17	0.45
3:D:1103:HIS:HA	3:D:1223:ILE:HD12	1.99	0.45
2:M:892:LEU:HD13	2:M:989:VAL:O	2.16	0.45
5:F:160:ASP:OD2	5:F:163:LEU:HD12	2.16	0.45
5:P:361:LEU:HD22	5:P:404:ALA:HB1	1.99	0.45
3:N:1428:ALA:C	3:N:1430:SER:H	2.20	0.45
3:D:213:VAL:HA	9:D:2673:HOH:O	2.16	0.45
3:D:777:PRO:HD2	3:D:912:LYS:HE2	1.97	0.45
2:C:1016:ILE:CD1	2:C:1016:ILE:H	2.20	0.45
2:C:164:PRO:HA	2:C:266:ARG:HH12	1.80	0.45
3:D:206:ARG:HB3	3:D:206:ARG:NH1	2.32	0.45
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.97	0.45
2:C:580:MET:HB3	9:C:2049:HOH:O	2.16	0.45
3:D:452:ILE:HG23	3:D:452:ILE:O	2.17	0.45
2:M:84:ARG:HH12	2:M:128:ILE:HG12	1.78	0.45
5:P:217:ASN:O	5:P:220:LEU:HB3	2.16	0.45
3:N:572:ARG:O	3:N:575:GLN:HB3	2.17	0.45
3:N:1195:GLN:HG3	9:N:2116:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:250:ARG:HD2	9:M:9919:HOH:O	2.17	0.45
3:D:1256:LEU:HB3	3:D:1257:PRO:HD3	1.98	0.45
1:L:153:ALA:HA	1:L:156:HIS:CE1	2.51	0.45
2:C:1081:VAL:HB	2:C:1086:ARG:NH2	2.31	0.45
4:O:29:GLN:HB2	4:O:33:HIS:HD2	1.81	0.45
1:A:20:TYR:HE2	1:A:198:ARG:HB3	1.81	0.45
2:M:799:ILE:HD13	2:M:799:ILE:H	1.81	0.45
3:N:1359:GLN:HB3	3:N:1359:GLN:HE21	1.49	0.45
2:C:475:VAL:HA	9:C:9621:HOH:O	2.16	0.45
3:N:988:ARG:HD2	3:N:992:ILE:CD1	2.46	0.45
2:C:505:GLY:HA3	9:C:9589:HOH:O	2.17	0.45
3:D:908:LYS:NZ	8:N:9100:G4P:O2D	2.49	0.45
3:N:179:VAL:HG11	9:N:2712:HOH:O	2.17	0.45
3:D:148:GLU:N	3:D:148:GLU:CD	2.70	0.45
2:C:1083:GLU:O	2:C:1087:VAL:HG23	2.16	0.45
2:M:288:ARG:NH1	2:M:289:THR:HG23	2.31	0.45
2:M:327:HIS:ND1	2:M:433:THR:HG21	2.32	0.45
2:C:202:TYR:CZ	2:C:304:LEU:HD22	2.51	0.45
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.44	0.45
2:C:151:ASP:OD1	2:C:152:PRO:HD2	2.17	0.45
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.99	0.45
2:M:1088:LEU:O	2:M:1091:GLU:HB2	2.17	0.45
2:C:717:LEU:HD11	2:C:764:GLU:O	2.16	0.45
3:N:1194:CYS:SG	3:N:1200:VAL:HA	2.57	0.45
1:B:207:PRO:HD2	9:B:9568:HOH:O	2.17	0.45
2:M:395:LYS:HE3	2:M:407:LYS:HZ2	1.82	0.45
2:M:407:LYS:HG2	9:M:9254:HOH:O	2.15	0.45
3:N:631:ILE:HG21	3:N:745:MET:HG3	1.97	0.45
3:N:1312:LEU:HG	3:N:1327:ARG:HG3	1.99	0.45
2:C:777:ILE:HG23	9:C:9997:HOH:O	2.16	0.45
3:N:813:LEU:O	3:N:817:GLU:HB2	2.15	0.45
3:D:808:THR:HB	3:D:809:PRO:HD3	1.97	0.45
1:A:219:ARG:HG2	9:A:9621:HOH:O	2.17	0.45
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.98	0.45
2:M:713:ARG:HD2	9:M:9901:HOH:O	2.17	0.45
2:M:172:ILE:HA	2:M:185:LYS:O	2.16	0.45
5:P:166:LEU:HD13	5:P:170:HIS:CB	2.47	0.45
3:N:1433:SER:HB2	3:N:1457:ASP:OD1	2.17	0.45
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.15	0.45
2:M:575:GLN:H	2:M:667:ALA:HB1	1.81	0.45
2:M:501:THR:O	2:M:503:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:ARG:HD2	9:D:9624:HOH:O	2.17	0.45
3:N:964:LEU:O	3:N:968:ASP:HB2	2.17	0.45
3:D:441:ARG:O	3:D:443:VAL:N	2.44	0.45
3:N:1241:PHE:O	3:N:1257:PRO:HB3	2.17	0.45
3:D:196:VAL:HG13	3:D:202:VAL:HG13	1.98	0.45
1:B:228:PRO:HG2	9:B:9723:HOH:O	2.15	0.45
2:C:262:ALA:HB2	9:C:2720:HOH:O	2.15	0.45
3:N:1017:PHE:HZ	9:N:9258:HOH:O	1.98	0.45
3:D:1460:ILE:HA	9:D:2240:HOH:O	2.17	0.45
3:D:586:ARG:HD2	9:D:2072:HOH:O	2.17	0.45
3:D:986:ARG:NH1	3:D:986:ARG:HB2	2.32	0.45
4:O:40:LEU:HB2	4:O:45:ARG:CD	2.46	0.45
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.52	0.45
3:N:1425:THR:O	3:N:1429:LEU:HD13	2.17	0.45
3:N:177:ALA:C	3:N:199:LEU:HD13	2.37	0.45
3:N:824:ASN:O	3:N:826:PRO:HD3	2.17	0.45
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.98	0.45
3:N:448:GLU:H	3:N:448:GLU:CD	2.20	0.45
3:D:972:LEU:CG	3:D:976:GLN:HE22	2.23	0.45
3:D:570:GLU:OE2	5:F:214:GLN:HG3	2.16	0.45
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.99	0.45
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.99	0.45
1:B:13:VAL:HG11	1:B:208:LEU:HD21	1.99	0.45
2:M:1031:ARG:HB3	9:N:9740:HOH:O	2.16	0.45
2:M:404:LEU:CD2	2:M:587:VAL:HG13	2.47	0.45
1:L:176:ARG:HH12	3:N:884:ARG:CZ	2.29	0.45
2:M:709:GLU:CD	2:M:824:ARG:HG2	2.38	0.45
3:D:867:ARG:HG3	9:D:2678:HOH:O	2.16	0.45
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.46	0.45
1:A:22:GLU:N	9:A:9810:HOH:O	2.49	0.45
4:E:41:GLU:HB3	4:E:42:PRO:HD3	1.98	0.45
3:N:701:LEU:O	3:N:702:LEU:HD12	2.16	0.45
1:A:53:VAL:HG21	1:A:82:LEU:HB3	1.99	0.45
5:P:171:LYS:HG2	5:P:175:HIS:CE1	2.52	0.45
2:M:745:ILE:HG12	9:M:9460:HOH:O	2.17	0.45
5:F:257:THR:C	5:F:258:ILE:HG13	2.37	0.45
2:M:20:GLU:O	2:M:24:GLU:HB2	2.16	0.45
2:C:958:THR:CG2	2:C:961:GLU:HB2	2.46	0.45
3:N:792:ILE:O	3:N:878:GLY:HA3	2.17	0.45
3:N:1390:LEU:HD13	9:N:9981:HOH:O	2.17	0.45
2:C:1081:VAL:HB	2:C:1086:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:LEU:HD12	1:L:3:ASP:H	1.82	0.45
5:F:376:ILE:HG22	9:F:9780:HOH:O	2.16	0.45
3:D:175:VAL:HG11	9:D:9726:HOH:O	2.17	0.45
3:D:792:ILE:HD12	3:D:941:PHE:CE1	2.52	0.45
3:N:590:PRO:HD2	9:N:9686:HOH:O	2.16	0.45
1:L:166:PRO:HB2	9:L:3282:HOH:O	2.16	0.45
3:D:95:LEU:HA	9:D:2002:HOH:O	2.17	0.45
2:C:676:ILE:HG22	2:C:988:VAL:O	2.17	0.45
3:D:170:PRO:O	3:D:391:ALA:HB3	2.17	0.45
3:D:1046:GLN:HB3	3:D:1052:THR:CG2	2.47	0.45
2:C:672:VAL:HG23	2:C:868:ASP:OD2	2.17	0.45
3:N:693:GLU:HG3	4:O:48:MET:HE3	1.98	0.45
2:C:838:LYS:HD2	2:C:846:LYS:HZ3	1.81	0.45
2:M:397:GLU:H	2:M:633:GLN:NE2	2.14	0.45
2:C:612:VAL:HG22	2:C:622:GLU:CA	2.46	0.45
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.82	0.45
2:M:455:LEU:HD22	2:M:459:ALA:HB1	1.98	0.45
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.98	0.45
4:O:32:ARG:C	4:O:34:GLY:H	2.20	0.45
2:M:673:LEU:HD13	9:M:9318:HOH:O	2.16	0.45
5:F:96:LEU:O	5:F:100:VAL:HG23	2.17	0.45
3:N:469:ASP:OD1	3:N:471:GLU:HB2	2.17	0.45
1:B:68:ILE:HG23	9:B:9743:HOH:O	2.16	0.45
3:D:1005:GLN:HB2	9:D:9713:HOH:O	2.16	0.45
3:D:833:GLU:HB2	9:D:2078:HOH:O	2.16	0.45
3:D:561:GLY:HA2	9:D:9763:HOH:O	2.17	0.45
3:D:216:VAL:HG12	9:D:9564:HOH:O	2.17	0.45
5:P:306:GLU:O	5:P:310:ILE:HG13	2.17	0.45
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.81	0.45
5:F:151:LEU:HB2	5:F:155:THR:OG1	2.17	0.45
2:M:35:PRO:HD2	2:M:38:LYS:HG2	1.99	0.45
3:N:133:ILE:HD11	3:N:456:MET:HE3	1.99	0.45
3:N:789:LEU:HD12	3:N:911:LEU:HD21	1.98	0.45
3:N:161:LEU:HG	3:N:449:SER:OG	2.17	0.45
3:D:1141:GLU:O	3:D:1145:TYR:HB2	2.17	0.45
2:C:764:GLU:HG3	9:F:9714:HOH:O	2.16	0.45
5:P:150:THR:HG23	5:P:155:THR:CG2	2.46	0.45
2:C:1014:SER:OG	5:F:331:ASP:HA	2.17	0.45
5:F:84:TYR:HD2	5:F:192:LEU:HD13	1.82	0.45
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.17	0.45
5:F:125:ASP:O	5:F:129:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:TYR:CD2	1:K:161:ARG:HD3	2.52	0.45
3:N:1459:LEU:HB3	3:N:1465:ASN:HD22	1.82	0.45
2:C:404:LEU:HA	2:C:407:LYS:HZ3	1.81	0.45
3:D:161:LEU:O	3:D:449:SER:HB2	2.17	0.45
1:B:176:ARG:HB3	9:B:9633:HOH:O	2.16	0.45
2:C:881:ASN:H	2:C:881:ASN:ND2	2.14	0.45
5:P:77:THR:HA	9:P:1606:HOH:O	2.17	0.45
2:M:955:PRO:HD3	9:M:9923:HOH:O	2.17	0.45
2:M:742:VAL:HG12	2:M:743:VAL:N	2.32	0.45
2:C:650:ARG:HG3	9:C:9988:HOH:O	2.17	0.45
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.47	0.44
2:M:276:LYS:HG3	9:M:9544:HOH:O	2.16	0.44
5:F:295:MET:HE2	5:F:295:MET:HA	1.99	0.44
3:N:829:VAL:HA	9:N:9979:HOH:O	2.17	0.44
2:C:257:VAL:C	2:C:259:GLY:H	2.21	0.44
3:D:844:ALA:O	3:D:867:ARG:HB3	2.17	0.44
1:L:213:GLN:HG3	9:L:1267:HOH:O	2.17	0.44
3:N:1031:ASN:O	3:N:1034:GLN:HB2	2.17	0.44
1:L:49:PRO:HA	1:L:148:VAL:HG12	2.00	0.44
3:D:12:LEU:HD21	3:D:104:PHE:CE1	2.52	0.44
9:N:9941:HOH:O	5:P:312:GLN:HB3	2.16	0.44
2:M:927:GLY:HA2	2:M:930:LYS:HZ2	1.81	0.44
2:C:895:TYR:HD1	2:C:991:GLN:HE21	1.64	0.44
5:F:153:PRO:CG	5:F:154:LYS:H	2.30	0.44
3:D:59:ALA:HB2	9:D:2190:HOH:O	2.17	0.44
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.99	0.44
3:D:441:ARG:HB3	3:D:443:VAL:HG23	1.98	0.44
2:C:134:ARG:HG3	2:C:393:GLN:O	2.17	0.44
3:D:416:ALA:HB3	3:D:417:PRO:HD3	1.99	0.44
5:P:413:SER:HA	9:P:2117:HOH:O	2.16	0.44
3:N:903:ASP:HA	9:N:9960:HOH:O	2.17	0.44
3:D:35:ARG:HD3	9:D:2024:HOH:O	2.17	0.44
3:D:956:ILE:HB	9:D:2735:HOH:O	2.18	0.44
5:P:287:THR:CG2	5:P:289:GLU:HB2	2.43	0.44
5:F:134:LYS:NZ	5:F:160:ASP:HB2	2.31	0.44
3:D:699:VAL:HB	3:D:716:PHE:O	2.18	0.44
2:C:64:LEU:HD13	2:C:359:MET:CG	2.47	0.44
5:F:274:THR:O	5:F:278:LEU:HG	2.18	0.44
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.33	0.44
3:N:1109:GLU:CG	3:N:1201:CYS:HA	2.38	0.44
1:A:181:VAL:HG12	9:C:9642:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:LEU:HD22	3:D:195:VAL:HG11	1.99	0.44
3:D:177:ALA:CA	3:D:199:LEU:HD13	2.46	0.44
2:M:906:PHE:CZ	3:N:1067:VAL:HA	2.52	0.44
3:N:141:ILE:HD12	3:N:141:ILE:N	2.26	0.44
3:N:724:GLN:HA	9:N:9508:HOH:O	2.17	0.44
4:E:54:LEU:HG	4:E:58:PRO:CG	2.47	0.44
2:M:302:VAL:HG13	2:M:303:PHE:N	2.32	0.44
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.97	0.44
2:M:64:LEU:HD22	2:M:359:MET:CG	2.43	0.44
2:M:759:THR:N	9:M:9349:HOH:O	2.44	0.44
2:C:172:ILE:H	2:C:172:ILE:HD12	1.82	0.44
3:N:130:SER:HA	3:N:572:ARG:HH12	1.82	0.44
3:N:893:GLU:O	3:N:896:ALA:HB3	2.17	0.44
2:M:1105:LYS:O	2:M:1107:ASN:N	2.50	0.44
3:D:1149:LEU:HD11	3:D:1160:LEU:HB3	2.00	0.44
3:N:42:ASP:HB2	9:N:9477:HOH:O	2.16	0.44
3:N:472:ALA:HA	9:N:9220:HOH:O	2.18	0.44
3:D:1260:ILE:HG21	9:D:2566:HOH:O	2.17	0.44
2:M:301:GLU:HA	9:M:2582:HOH:O	2.17	0.44
3:N:689:ASP:HB3	9:O:1346:HOH:O	2.17	0.44
2:M:918:LEU:HD12	2:M:918:LEU:HA	1.85	0.44
3:D:186:VAL:HG13	3:D:187:LYS:N	2.32	0.44
3:N:427:VAL:HG13	9:N:9378:HOH:O	2.16	0.44
3:N:481:MET:SD	3:N:1388:ARG:HG2	2.57	0.44
2:M:119:PRO:HB2	9:M:9763:HOH:O	2.16	0.44
5:F:300:ASP:O	5:F:304:VAL:HG23	2.17	0.44
4:E:13:VAL:HG11	4:E:19:LEU:HB2	1.99	0.44
2:C:742:VAL:HG12	2:C:743:VAL:N	2.31	0.44
3:N:452:ILE:HG21	9:N:9295:HOH:O	2.17	0.44
1:K:92:PRO:HB2	9:K:1355:HOH:O	2.15	0.44
2:C:65:VAL:HG12	2:C:67:ASP:OD1	2.16	0.44
2:M:436:GLY:O	2:M:469:THR:HB	2.17	0.44
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.16	0.44
2:C:147:TYR:HE2	2:C:330:ASN:OD1	1.99	0.44
2:C:327:HIS:HE2	2:C:492:ASP:CG	2.21	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HD3	1.99	0.44
1:L:132:LEU:HD22	9:L:4720:HOH:O	2.17	0.44
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.46	0.44
3:D:1068:LEU:O	3:D:1069:GLU:C	2.55	0.44
1:B:206:THR:CG2	1:B:209:GLU:H	2.29	0.44
3:N:712:GLY:HA3	9:N:2395:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:224:GLU:HB3	2:M:227:PHE:CD1	2.52	0.44
2:C:439:CYS:SG	2:C:540:PHE:HB3	2.57	0.44
2:C:798:GLY:H	2:C:827:VAL:HG11	1.81	0.44
3:D:1498:ALA:HA	9:E:9588:HOH:O	2.17	0.44
3:D:881:LEU:HD11	3:D:884:ARG:HH21	1.81	0.44
3:D:789:LEU:HD22	3:D:882:PHE:CE1	2.52	0.44
3:N:549:ASN:ND2	5:P:254:GLN:HE21	2.16	0.44
4:E:85:LEU:HA	9:E:9561:HOH:O	2.17	0.44
9:K:2274:HOH:O	2:M:865:THR:HG22	2.16	0.44
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.52	0.44
3:D:1110:ALA:HB1	9:D:2073:HOH:O	2.17	0.44
3:D:422:ALA:O	3:D:427:VAL:HG21	2.18	0.44
3:D:500:ARG:HH22	3:D:1388:ARG:NE	2.15	0.44
2:M:418:LEU:HB2	9:M:2268:HOH:O	2.16	0.44
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.48	0.44
5:F:291:ILE:HG23	5:F:292:ALA:N	2.32	0.44
3:N:983:LEU:HD13	9:N:9836:HOH:O	2.17	0.44
3:D:210:ARG:HG3	9:D:9645:HOH:O	2.17	0.44
1:K:133:GLU:N	9:K:1268:HOH:O	2.50	0.44
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	2.00	0.44
2:M:1015:LEU:HA	5:P:335:ASP:HB2	1.99	0.44
1:B:86:VAL:HG23	9:B:9660:HOH:O	2.17	0.44
2:C:480:THR:HG22	2:C:482:GLU:H	1.83	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.52	0.44
1:K:12:THR:HG21	9:K:1709:HOH:O	2.16	0.44
2:C:254:VAL:HG22	2:C:258:TYR:HE1	1.81	0.44
3:D:450:TYR:HB3	9:D:2159:HOH:O	2.17	0.44
2:C:127:PHE:O	2:C:133:ASP:HA	2.17	0.44
2:C:516:ARG:NH1	3:D:1068:LEU:HD22	2.32	0.44
5:P:113:ILE:HD12	9:P:4659:HOH:O	2.18	0.44
2:C:209:ARG:O	2:C:213:ALA:HB2	2.17	0.44
2:C:926:PHE:O	2:C:929:ARG:HB2	2.17	0.44
2:M:928:LYS:HE2	2:M:928:LYS:HA	1.99	0.44
3:N:500:ARG:NH1	3:N:500:ARG:HG3	2.33	0.44
3:D:814:ALA:HB2	9:D:2210:HOH:O	2.17	0.44
2:C:631:SER:HB3	2:C:637:LEU:HD22	2.00	0.44
2:C:816:LYS:O	2:C:819:VAL:HB	2.18	0.44
3:N:864:VAL:HG12	3:N:865:THR:H	1.82	0.44
2:C:930:LYS:HD3	2:C:960:GLU:OE1	2.18	0.44
3:N:192:ALA:HB3	9:N:9235:HOH:O	2.18	0.44
3:D:1382:THR:O	3:D:1384:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:777:ILE:HG22	2:M:778:PHE:N	2.31	0.44
3:N:513:ILE:H	3:N:513:ILE:HG13	1.65	0.44
3:D:186:VAL:HG23	3:D:211:VAL:CG1	2.48	0.44
3:D:907:GLU:O	3:D:911:LEU:HD13	2.18	0.44
2:M:1067:TYR:CD2	5:P:345:ALA:HB2	2.53	0.44
2:C:560:MET:O	2:C:564:MET:HB2	2.17	0.44
3:D:1341:PRO:HA	3:D:1344:VAL:CG2	2.46	0.44
2:M:598:GLU:N	9:M:9609:HOH:O	2.50	0.44
3:N:808:THR:HB	3:N:809:PRO:HD3	1.98	0.44
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.18	0.44
3:N:767:HIS:C	3:N:768:ASN:HD22	2.20	0.44
9:A:9736:HOH:O	1:B:156:HIS:HB3	2.18	0.44
3:N:796:ARG:NE	3:N:828:LYS:HZ3	2.15	0.44
3:N:1277:ILE:CG2	3:N:1278:ASP:N	2.80	0.44
2:M:21:ILE:HD12	2:M:21:ILE:N	2.30	0.44
1:K:30:ARG:HH22	1:L:155:LYS:NZ	2.16	0.44
2:C:45:GLN:NE2	9:C:2296:HOH:O	2.49	0.44
1:B:206:THR:HG22	1:B:209:GLU:CG	2.48	0.44
2:C:899:GLN:HA	9:C:2768:HOH:O	2.17	0.44
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.47	0.44
2:M:1095:LEU:HD23	3:N:582:LEU:HD23	1.99	0.44
3:N:101:HIS:CD2	3:N:582:LEU:HD22	2.52	0.44
3:D:1393:GLN:HB3	9:D:9676:HOH:O	2.17	0.44
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.47	0.44
2:M:432:ARG:HG3	2:M:432:ARG:HH11	1.82	0.44
2:M:49:ARG:HB2	9:M:9976:HOH:O	2.17	0.44
1:K:83:LYS:HD3	9:K:2976:HOH:O	2.18	0.44
1:L:113:ASP:HA	9:L:1552:HOH:O	2.18	0.44
2:M:8:ARG:HG3	9:M:9876:HOH:O	2.17	0.44
2:C:188:LYS:C	2:C:188:LYS:HD3	2.37	0.44
3:N:619:LEU:O	3:N:619:LEU:HD23	2.18	0.44
2:M:1008:ARG:HG2	2:M:1008:ARG:HH11	1.82	0.44
1:B:79:ILE:HA	1:B:82:LEU:HD12	2.00	0.44
2:M:860:HIS:CE1	2:M:977:GLY:HA2	2.51	0.44
1:A:95:GLN:HB3	9:A:9602:HOH:O	2.17	0.44
4:E:50:THR:HG23	9:E:9582:HOH:O	2.16	0.44
2:C:321:GLU:HG3	9:C:2328:HOH:O	2.18	0.44
1:K:42:ARG:CZ	9:K:4396:HOH:O	2.65	0.44
2:M:31:GLN:HE21	2:M:31:GLN:HB3	1.50	0.44
3:D:87:ARG:HD2	3:D:88:TYR:CE2	2.53	0.44
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:85:VAL:O	3:N:89:ARG:HG3	2.18	0.44
2:M:676:ILE:HG22	2:M:988:VAL:O	2.17	0.44
4:E:23:VAL:HG11	9:E:9593:HOH:O	2.18	0.44
2:M:492:ASP:HA	9:M:9579:HOH:O	2.18	0.44
2:C:811:PRO:HD2	2:C:813:VAL:HG13	1.99	0.44
3:N:768:ASN:HD22	3:N:768:ASN:N	2.15	0.44
4:O:70:THR:HG22	4:O:71:GLY:H	1.83	0.44
3:D:835:SER:HB3	9:D:2297:HOH:O	2.16	0.44
1:L:77:GLU:HG3	9:N:2080:HOH:O	2.18	0.44
5:P:266:GLU:HB2	5:P:270:LYS:HZ3	1.80	0.44
1:K:189:ARG:HG2	1:K:190:THR:N	2.33	0.44
2:M:893:ALA:O	2:M:897:LEU:HB2	2.16	0.44
3:N:38:LYS:HG3	9:N:9685:HOH:O	2.16	0.44
3:D:470:LEU:HB3	3:D:503:LEU:HD11	2.00	0.44
1:B:10:VAL:HA	9:B:9606:HOH:O	2.17	0.44
2:M:799:ILE:O	2:M:801:VAL:HG13	2.17	0.44
2:M:860:HIS:HA	2:M:866:PRO:HA	1.99	0.44
2:M:563:ASN:HA	9:M:9240:HOH:O	2.16	0.44
3:N:1417:TRP:HD1	9:N:9725:HOH:O	2.00	0.44
1:K:31:GLY:N	1:K:193:ASP:OD1	2.51	0.44
3:D:986:ARG:HH11	3:D:986:ARG:HB2	1.83	0.44
3:N:12:LEU:CD2	3:N:13:ALA:H	2.30	0.44
3:N:18:ILE:HG21	3:N:516:ALA:O	2.17	0.44
3:D:1470:ARG:HG2	3:D:1471:LEU:N	2.32	0.44
2:M:288:ARG:HH12	2:M:289:THR:HG23	1.82	0.44
2:M:338:GLU:HA	2:M:341:THR:CG2	2.44	0.44
3:D:168:THR:HG22	3:D:170:PRO:HD3	2.00	0.44
3:N:1384:PRO:HG3	3:N:1389:LEU:N	2.33	0.44
3:N:895:VAL:O	3:N:899:LEU:HD12	2.17	0.44
5:P:339:PRO:HA	9:P:1420:HOH:O	2.18	0.44
1:L:80:LEU:HD13	3:N:842:VAL:CG1	2.42	0.44
2:C:584:GLU:HB2	2:C:666:LEU:H	1.83	0.44
2:C:1021:LEU:HD13	5:F:331:ASP:O	2.18	0.44
2:M:545:ASN:HD21	2:M:905:ILE:HG13	1.82	0.44
3:N:441:ARG:HD2	9:N:9328:HOH:O	2.18	0.44
1:K:97:VAL:HG11	1:K:120:VAL:HG21	1.99	0.44
4:E:91:ARG:CZ	9:E:9574:HOH:O	2.66	0.44
1:K:41:ARG:HG3	1:K:41:ARG:HH11	1.83	0.44
3:D:563:PRO:HG3	5:F:188:ILE:CG2	2.47	0.44
3:N:138:LYS:H	3:N:138:LYS:CD	2.31	0.44
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:994:GLN:HE21	3:N:998:GLU:CD	2.20	0.44
1:L:14:ARG:HH22	1:L:24:VAL:CG2	2.31	0.44
3:N:1487:VAL:CG1	3:N:1488:ASP:N	2.81	0.44
2:C:607:ASP:HB2	2:C:610:ARG:H	1.81	0.44
1:B:26:GLU:CB	1:B:194:LYS:HG3	2.48	0.44
2:C:639:GLN:HB3	2:C:656:ALA:HB1	2.00	0.44
3:N:1162:GLU:HB3	9:N:9990:HOH:O	2.18	0.44
3:D:1101:VAL:CG1	3:D:1427:SER:HB3	2.46	0.44
3:N:1397:LYS:HG2	9:N:2363:HOH:O	2.17	0.44
3:D:82:LYS:O	3:D:84:ILE:N	2.51	0.44
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.99	0.44
3:D:116:LEU:HB3	3:D:118:LEU:CD1	2.44	0.44
3:D:130:SER:CB	3:D:572:ARG:HH12	2.30	0.44
3:N:1145:TYR:HA	9:N:2585:HOH:O	2.17	0.44
3:N:396:VAL:HG13	3:N:447:VAL:HA	2.00	0.44
5:F:111:GLU:O	5:F:115:LYS:HG3	2.18	0.44
2:M:872:ASN:OD1	2:M:874:LEU:N	2.47	0.44
2:C:517:ARG:O	2:C:519:GLY:N	2.51	0.44
2:C:1052:MET:HG3	3:D:623:VAL:HG21	1.98	0.44
1:L:176:ARG:HH22	3:N:884:ARG:HE	1.65	0.44
1:K:72:LYS:HZ1	2:M:644:VAL:HG12	1.82	0.44
2:M:303:PHE:HZ	9:M:2121:HOH:O	2.00	0.44
4:O:70:THR:HG22	4:O:71:GLY:N	2.33	0.44
4:E:51:LEU:HD21	9:E:9611:HOH:O	2.17	0.44
3:N:1192:LEU:N	9:N:9676:HOH:O	2.50	0.44
2:M:1081:VAL:HB	2:M:1086:ARG:NE	2.32	0.44
2:C:250:ARG:HD2	9:C:2643:HOH:O	2.17	0.44
3:N:70:GLY:C	3:N:71:LYS:HD2	2.38	0.44
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.83	0.44
3:D:1044:LEU:N	9:D:2029:HOH:O	2.51	0.44
3:D:36:THR:O	3:D:38:LYS:N	2.50	0.44
2:C:456:ALA:HA	2:C:541:SER:HA	1.98	0.44
3:D:937:TYR:HA	3:D:940:THR:OG1	2.18	0.44
2:C:913:GLU:HB3	9:C:2225:HOH:O	2.17	0.44
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.47	0.44
3:N:606:ILE:HG21	9:N:2854:HOH:O	2.18	0.44
3:D:697:GLY:HA3	4:E:59:ASN:OD1	2.17	0.44
3:D:964:LEU:O	3:D:968:ASP:HB2	2.18	0.44
3:N:205:TYR:N	3:N:205:TYR:CD1	2.86	0.44
5:P:361:LEU:HD21	5:P:408:LEU:HB2	1.99	0.44
2:M:31:GLN:NE2	2:M:34:VAL:HG23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:31:GLN:OE1	2:M:40:GLU:HB2	2.16	0.44
2:M:272:ALA:HB1	9:M:9251:HOH:O	2.17	0.44
2:M:50:GLU:OE2	2:M:345:ARG:HD2	2.18	0.44
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.48	0.44
2:M:130:ASN:HB3	9:M:9773:HOH:O	2.18	0.44
5:F:315:VAL:HG12	5:F:316:SER:H	1.83	0.44
2:C:129:ILE:HG22	2:C:130:ASN:H	1.83	0.44
3:D:1197:ARG:HG3	3:D:1198:TYR:N	2.33	0.44
2:M:588:VAL:HG23	2:M:596:TYR:OH	2.18	0.44
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.48	0.44
3:N:1147:ARG:HD2	3:N:1188:VAL:CG2	2.48	0.44
2:C:365:ASP:O	2:C:367:LEU:HD23	2.18	0.44
2:C:720:GLU:HA	2:C:759:THR:O	2.18	0.44
2:M:747:ALA:HB1	9:M:9356:HOH:O	2.17	0.44
3:N:1459:LEU:HD13	3:N:1465:ASN:HA	1.99	0.44
2:C:823:VAL:HG22	9:C:9907:HOH:O	2.18	0.44
3:D:1036:ARG:NH1	9:D:9667:HOH:O	2.51	0.44
5:F:187:LEU:HD23	5:F:191:ASN:HD22	1.82	0.44
3:D:395:VAL:O	3:D:395:VAL:HG12	2.18	0.44
2:C:896:PHE:HB2	9:C:2761:HOH:O	2.18	0.44
2:C:929:ARG:NH1	2:C:929:ARG:HG3	2.33	0.44
1:K:227:ASN:HB2	9:K:1432:HOH:O	2.17	0.44
5:F:259:ARG:HG2	5:F:259:ARG:NH1	2.32	0.44
2:M:798:GLY:H	2:M:827:VAL:HG11	1.82	0.44
3:D:953:ASP:OD1	3:D:1019:PRO:HG2	2.18	0.44
3:N:196:VAL:HG13	3:N:202:VAL:HG13	1.99	0.44
2:C:749:VAL:HG23	2:C:749:VAL:O	2.18	0.44
5:F:353:GLU:HA	9:F:9676:HOH:O	2.17	0.44
2:C:167:LYS:C	2:C:169:GLY:H	2.21	0.44
3:D:1244:GLY:HA3	9:D:2849:HOH:O	2.17	0.44
2:C:440:PRO:HD2	9:C:2264:HOH:O	2.18	0.44
2:C:789:SER:HB2	9:C:9581:HOH:O	2.18	0.44
3:N:172:PRO:CG	3:N:178:LEU:HD22	2.40	0.43
2:M:918:LEU:HD23	2:M:968:LEU:O	2.17	0.43
3:N:65:ARG:HD3	3:N:66:GLN:N	2.31	0.43
3:D:154:THR:HG22	3:D:155:ASP:N	2.32	0.43
2:C:941:VAL:O	2:C:944:LEU:HB2	2.18	0.43
5:F:288:TYR:CE2	5:F:305:GLU:HA	2.52	0.43
3:N:984:THR:HB	3:N:987:GLU:OE1	2.18	0.43
2:M:192:PRO:HB3	2:M:194:VAL:HG23	1.99	0.43
5:F:113:ILE:HG23	5:F:127:ILE:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:966:GLU:HG3	9:D:2760:HOH:O	2.17	0.43
3:D:562:ALA:CB	3:D:567:ILE:HD11	2.40	0.43
3:D:1394:VAL:CG2	3:D:1397:LYS:HD2	2.47	0.43
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.52	0.43
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.39	0.43
3:N:1326:THR:HG21	9:N:2275:HOH:O	2.18	0.43
2:C:773:LEU:HA	9:C:9824:HOH:O	2.18	0.43
2:C:774:LEU:O	2:C:777:ILE:HB	2.18	0.43
1:B:85:LEU:HD12	1:B:124:ASN:HB3	2.00	0.43
2:C:781:LYS:HD2	9:C:9791:HOH:O	2.17	0.43
3:N:142:LEU:HB3	9:N:9595:HOH:O	2.17	0.43
3:D:1314:LYS:HE2	9:D:3278:HOH:O	2.18	0.43
1:A:85:LEU:HD12	1:A:124:ASN:HB3	2.00	0.43
3:N:126:VAL:HG23	9:N:9692:HOH:O	2.18	0.43
3:N:1412:LYS:C	3:N:1414:PRO:HD3	2.39	0.43
2:C:860:HIS:HA	2:C:866:PRO:HA	1.99	0.43
2:M:286:SER:HB3	2:M:299:LYS:CE	2.47	0.43
2:M:292:ARG:HE	2:M:299:LYS:HZ2	1.65	0.43
2:M:768:THR:HG23	9:M:9276:HOH:O	2.17	0.43
5:P:222:ARG:HD2	5:P:242:TRP:CE3	2.54	0.43
3:D:1136:LYS:HB2	3:D:1139:ASP:OD2	2.18	0.43
2:C:610:ARG:HD2	9:C:9662:HOH:O	2.18	0.43
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.76	0.43
3:D:34:TYR:CD1	3:D:35:ARG:N	2.86	0.43
4:E:29:GLN:HG3	9:E:9594:HOH:O	2.18	0.43
3:D:653:PHE:CD1	3:D:653:PHE:N	2.86	0.43
3:D:767:HIS:C	3:D:768:ASN:HD22	2.22	0.43
2:C:431:HIS:CD2	2:C:433:THR:H	2.36	0.43
3:D:1209:LEU:HD11	4:E:16:LYS:NZ	2.33	0.43
3:N:1046:GLN:CA	3:N:1052:THR:HA	2.37	0.43
2:M:208:ALA:HB3	2:M:209:ARG:HH21	1.83	0.43
5:F:164:LYS:HD2	9:F:9652:HOH:O	2.18	0.43
3:D:1374:GLN:OE1	3:D:1377:LYS:HD3	2.18	0.43
2:M:1015:LEU:HD12	5:P:333:ILE:CG2	2.48	0.43
1:L:78:ILE:O	1:L:82:LEU:HG	2.18	0.43
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.83	0.43
2:M:1031:ARG:HA	3:N:621:LYS:O	2.17	0.43
3:D:1063:GLU:HG2	3:D:1064:GLY:N	2.29	0.43
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.18	0.43
1:K:11:PHE:HB2	9:L:2122:HOH:O	2.17	0.43
3:N:759:ALA:O	3:N:763:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:404:ALA:O	5:F:408:LEU:HB2	2.19	0.43
1:L:106:PRO:HA	1:L:132:LEU:O	2.18	0.43
2:C:250:ARG:HH21	2:C:254:VAL:N	2.14	0.43
2:C:183:SER:HA	2:C:190:LYS:HB2	1.99	0.43
3:N:995:LEU:HA	3:N:998:GLU:OE1	2.18	0.43
2:M:243:ARG:HB3	9:M:9892:HOH:O	2.18	0.43
3:D:395:VAL:HB	9:D:9923:HOH:O	2.18	0.43
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.18	0.43
2:C:614:ARG:HG3	9:C:9611:HOH:O	2.18	0.43
2:M:444:PRO:CD	2:M:452:ILE:HG13	2.48	0.43
3:N:822:ALA:HB2	9:N:9525:HOH:O	2.18	0.43
5:F:207:LEU:HD12	5:F:212:LEU:CD2	2.48	0.43
4:E:70:THR:HG22	4:E:71:GLY:N	2.33	0.43
3:N:962:GLN:HA	9:N:9569:HOH:O	2.17	0.43
3:D:1499:ARG:HB3	9:D:2661:HOH:O	2.18	0.43
3:N:1303:TYR:HA	9:N:9699:HOH:O	2.18	0.43
5:P:192:LEU:HB3	9:P:4506:HOH:O	2.18	0.43
3:N:471:GLU:HG2	9:N:9786:HOH:O	2.17	0.43
3:N:647:ARG:HH12	3:N:680:GLN:HG3	1.82	0.43
5:P:289:GLU:HG2	9:P:4194:HOH:O	2.18	0.43
2:C:971:LYS:HG2	2:C:988:VAL:N	2.33	0.43
2:M:981:GLU:HA	9:M:9308:HOH:O	2.19	0.43
2:C:244:PRO:HD2	2:C:245:GLY:N	2.23	0.43
1:K:112:ARG:NH1	9:K:3292:HOH:O	2.50	0.43
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.99	0.43
2:C:840:ALA:HB2	2:C:846:LYS:HG3	1.99	0.43
2:M:597:ALA:O	2:M:652:GLY:N	2.50	0.43
2:M:569:VAL:O	2:M:571:LEU:HD12	2.17	0.43
4:E:48:MET:HB2	4:E:54:LEU:HD12	2.01	0.43
1:K:1:MET:O	1:K:6:LEU:HD22	2.18	0.43
2:C:12:VAL:CG1	2:C:534:VAL:HG13	2.48	0.43
3:N:759:ALA:HA	3:N:763:MET:HE1	2.00	0.43
1:K:24:VAL:HG22	1:K:196:THR:OG1	2.18	0.43
5:P:94:LEU:H	5:P:98:GLU:HB2	1.83	0.43
1:K:30:ARG:HD2	9:K:1388:HOH:O	2.17	0.43
3:N:873:LEU:HD23	9:N:2208:HOH:O	2.18	0.43
2:M:204:GLN:HE22	2:M:225:SER:HA	1.84	0.43
3:D:1406:ARG:NE	3:D:1412:LYS:HB3	2.33	0.43
3:D:719:VAL:HG11	9:D:9572:HOH:O	2.17	0.43
3:D:1425:THR:HB	9:D:9596:HOH:O	2.17	0.43
3:N:660:LYS:HD2	3:N:694:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:53:GLY:HA3	9:O:4631:HOH:O	2.17	0.43
3:N:380:GLU:HA	9:N:9923:HOH:O	2.18	0.43
3:D:1363:LEU:HD12	3:D:1363:LEU:O	2.19	0.43
2:C:115:LEU:HD12	2:C:378:LEU:CD2	2.48	0.43
1:A:97:VAL:HG11	1:A:120:VAL:HG21	1.99	0.43
1:B:83:LYS:HE2	1:B:167:VAL:HG12	2.00	0.43
2:M:163:ILE:O	2:M:163:ILE:HG23	2.17	0.43
3:D:123:LEU:O	3:D:126:VAL:HB	2.19	0.43
2:M:498:GLN:CG	2:M:516:ARG:HE	2.31	0.43
2:M:305:PRO:O	2:M:308:ARG:HB3	2.18	0.43
3:N:1147:ARG:H	3:N:1166:LEU:HG	1.83	0.43
2:C:336:VAL:HA	2:C:339:LEU:HD12	2.00	0.43
3:D:107:ASP:O	3:D:108:VAL:C	2.56	0.43
1:K:60:ASP:HA	9:K:3216:HOH:O	2.19	0.43
1:B:17:GLY:C	1:B:19:GLU:H	2.21	0.43
3:D:1310:ARG:HE	3:D:1310:ARG:HB2	1.69	0.43
2:C:881:ASN:HD22	2:C:881:ASN:N	2.12	0.43
3:D:193:PRO:HG3	9:D:3106:HOH:O	2.17	0.43
2:M:103:LYS:HG3	9:M:2256:HOH:O	2.19	0.43
2:M:250:ARG:HB2	2:M:253:ALA:CB	2.49	0.43
2:M:1105:LYS:HE3	9:M:9940:HOH:O	2.17	0.43
5:P:276:ARG:HD2	9:P:2013:HOH:O	2.16	0.43
2:C:802:ARG:HB2	9:C:9590:HOH:O	2.17	0.43
2:M:93:PRO:HB2	9:M:9852:HOH:O	2.19	0.43
2:M:999:HIS:HB3	2:M:1003:ASP:OD2	2.18	0.43
2:C:869:VAL:HG22	2:C:871:LEU:CD1	2.48	0.43
3:D:474:GLU:HG3	3:D:500:ARG:NE	2.32	0.43
3:D:523:ASP:HA	9:D:9853:HOH:O	2.18	0.43
3:D:460:ALA:O	3:D:464:LEU:HG	2.18	0.43
2:C:73:LEU:HB2	9:C:2521:HOH:O	2.19	0.43
2:C:139:GLN:HG2	2:C:140:ILE:H	1.83	0.43
3:N:459:GLU:OE2	5:P:144:ILE:HD12	2.19	0.43
2:C:256:TYR:HA	9:C:2199:HOH:O	2.17	0.43
5:F:273:ARG:HB3	9:F:9601:HOH:O	2.18	0.43
3:D:925:GLU:O	3:D:928:ALA:HB3	2.18	0.43
3:D:1197:ARG:HG2	9:D:2561:HOH:O	2.18	0.43
3:D:1397:LYS:HE2	9:D:3297:HOH:O	2.17	0.43
3:N:719:VAL:O	3:N:721:VAL:HG13	2.18	0.43
2:C:1014:SER:HA	5:F:333:ILE:O	2.18	0.43
2:M:14:PRO:HG3	9:M:2533:HOH:O	2.18	0.43
3:N:441:ARG:O	3:N:443:VAL:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:45:ARG:HB3	9:E:9659:HOH:O	2.18	0.43
3:D:994:GLN:HE21	3:D:998:GLU:CD	2.21	0.43
1:K:139:ASN:HB2	9:K:2209:HOH:O	2.18	0.43
2:M:1001:VAL:HG13	9:M:9394:HOH:O	2.17	0.43
2:M:575:GLN:HA	2:M:662:GLU:HG3	2.00	0.43
2:C:1034:GLU:HG3	2:C:1035:MET:H	1.83	0.43
2:C:144:PRO:HA	2:C:163:ILE:O	2.19	0.43
2:M:54:ILE:HD11	2:M:56:GLU:OE2	2.18	0.43
5:F:260:ILE:HG12	5:F:264:MET:HB2	2.01	0.43
3:N:1283:ILE:HG22	3:N:1284:GLU:N	2.34	0.43
3:N:30:GLU:HB3	3:N:40:GLU:CB	2.48	0.43
3:D:850:LEU:O	3:D:853:VAL:HB	2.18	0.43
2:C:27:ARG:HG3	9:C:9641:HOH:O	2.19	0.43
1:K:176:ARG:NH1	9:K:2274:HOH:O	2.50	0.43
5:P:253:ASP:HA	5:P:259:ARG:HE	1.83	0.43
5:P:356:LYS:O	5:P:360:LYS:HG2	2.18	0.43
3:N:1225:ALA:O	3:N:1229:ILE:HG13	2.18	0.43
3:D:1302:GLU:HG2	9:D:2309:HOH:O	2.18	0.43
2:M:811:PRO:HG3	9:M:9687:HOH:O	2.17	0.43
2:C:671:ASN:ND2	2:C:993:PHE:HD2	2.16	0.43
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.36	0.43
3:N:1080:GLY:O	3:N:1084:THR:HG23	2.19	0.43
2:C:218:VAL:HB	9:C:2262:HOH:O	2.18	0.43
3:N:422:ALA:HB2	9:N:9378:HOH:O	2.18	0.43
3:N:14:SER:OG	3:N:17:LYS:HB2	2.19	0.43
3:D:209:ARG:HB3	3:D:210:ARG:H	1.62	0.43
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.19	0.43
3:N:863:VAL:HA	9:N:9938:HOH:O	2.18	0.43
5:F:329:TYR:O	5:F:332:PHE:HB2	2.19	0.43
1:B:86:VAL:HA	9:B:9736:HOH:O	2.18	0.43
3:N:812:ALA:O	3:N:816:HIS:HB2	2.19	0.43
1:B:50:GLY:HA2	9:B:9569:HOH:O	2.18	0.43
3:N:796:ARG:NE	3:N:862:ASP:OD2	2.51	0.43
2:M:1086:ARG:NH1	9:M:9565:HOH:O	2.52	0.43
2:M:627:ARG:HD3	9:M:2410:HOH:O	2.18	0.43
5:P:288:TYR:HE2	5:P:305:GLU:HA	1.84	0.43
2:C:897:LEU:HB2	9:C:9860:HOH:O	2.17	0.43
5:F:406:ARG:HA	5:F:409:LYS:HD3	2.01	0.43
2:M:247:PRO:HA	2:M:248:PRO:HD3	1.89	0.43
2:M:755:LEU:HD21	2:M:792:VAL:HG22	2.01	0.43
3:N:1161:GLU:HB3	9:N:9583:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:442:ASN:HA	9:D:2613:HOH:O	2.19	0.43
3:N:1320:GLU:N	3:N:1323:GLN:NE2	2.67	0.43
1:K:83:LYS:HZ1	1:K:168:ASP:HB2	1.84	0.43
4:E:50:THR:HA	9:E:9570:HOH:O	2.19	0.43
3:D:380:GLU:O	3:D:382:GLU:N	2.51	0.43
3:D:101:HIS:CD2	3:D:103:TRP:HB2	2.53	0.43
3:D:101:HIS:CD2	3:D:582:LEU:HD13	2.53	0.43
5:F:387:GLY:HA2	9:F:9617:HOH:O	2.18	0.43
3:N:1357:ARG:HB3	9:N:2893:HOH:O	2.18	0.43
3:D:484:PRO:HG3	9:D:3258:HOH:O	2.18	0.43
2:M:1085:PHE:HE1	2:M:1111:ILE:HG21	1.83	0.43
3:N:447:VAL:HG23	3:N:448:GLU:N	2.34	0.43
2:C:165:LEU:HB2	9:C:2287:HOH:O	2.18	0.43
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.86	0.43
9:D:2199:HOH:O	4:E:58:PRO:HA	2.19	0.43
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.49	0.43
5:F:419:ARG:HA	9:F:9727:HOH:O	2.18	0.43
2:C:358:ARG:HH12	2:C:374:ASN:CG	2.21	0.43
1:L:176:ARG:HG3	1:L:200:TRP:CE3	2.53	0.43
2:C:534:VAL:N	2:C:538:GLN:NE2	2.67	0.43
3:D:806:PHE:N	9:D:2133:HOH:O	2.50	0.43
4:E:45:ARG:HH22	4:E:72:ARG:HH21	1.66	0.43
3:N:1103:HIS:HA	3:N:1223:ILE:HD12	2.00	0.43
3:N:684:LYS:HE3	9:N:2460:HOH:O	2.18	0.43
3:N:137:PRO:HG2	9:N:2197:HOH:O	2.18	0.43
2:C:474:VAL:HB	2:C:479:VAL:HG12	1.99	0.43
5:F:402:ASN:HB3	9:F:9689:HOH:O	2.17	0.43
3:N:792:ILE:HG23	3:N:793:THR:N	2.32	0.43
3:N:19:ARG:HH21	3:N:94:GLU:CD	2.21	0.43
3:D:231:VAL:HA	3:D:378:ILE:CB	2.49	0.43
2:C:95:TYR:HE2	9:C:9699:HOH:O	2.01	0.43
1:L:55:SER:HB2	1:L:158:ILE:HB	2.01	0.43
5:F:153:PRO:O	5:F:157:GLU:HG3	2.18	0.43
4:O:6:ILE:HG23	4:O:7:ASP:N	2.33	0.43
1:L:47:SER:CB	1:L:217:ILE:HD13	2.48	0.43
3:D:1096:ARG:NH1	3:D:1096:ARG:HB2	2.33	0.43
5:F:142:ARG:HG3	9:F:2143:HOH:O	2.19	0.43
2:C:188:LYS:HE2	9:C:2731:HOH:O	2.18	0.43
3:D:960:LYS:HG2	3:D:964:LEU:CD1	2.49	0.43
3:D:968:ASP:O	3:D:971:LEU:HB3	2.19	0.43
1:L:227:ASN:HB2	9:L:1651:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG22	1:A:203:GLY:H	1.82	0.43
9:D:2183:HOH:O	5:F:349:LEU:HD13	2.19	0.43
2:M:854:PRO:HB2	2:M:856:GLU:HB2	2.00	0.43
3:D:1431:THR:HB	3:D:1432:LYS:HE3	1.99	0.43
2:C:64:LEU:HB2	2:C:359:MET:SD	2.59	0.43
2:M:42:VAL:HG13	2:M:268:ASP:OD2	2.18	0.43
3:D:155:ASP:HB3	9:D:2347:HOH:O	2.18	0.43
2:C:396:ASP:OD1	2:C:402:SER:HB3	2.18	0.43
5:F:291:ILE:CG2	5:F:304:VAL:HG21	2.48	0.43
5:P:342:VAL:HG23	5:P:343:ASP:N	2.34	0.43
4:O:47:LYS:C	4:O:54:LEU:HD13	2.39	0.43
2:C:520:GLU:HB2	9:C:9578:HOH:O	2.19	0.43
4:E:23:VAL:HG13	4:E:24:ALA:N	2.34	0.43
5:P:138:SER:N	9:P:2295:HOH:O	2.52	0.43
1:K:224:TYR:CD1	1:L:9:PRO:HD2	2.54	0.43
3:N:1166:LEU:HD23	3:N:1166:LEU:N	2.27	0.43
2:C:773:LEU:HD21	5:F:354:LEU:HD11	2.00	0.43
2:C:274:ARG:N	2:C:288:ARG:HH22	2.17	0.43
2:M:790:LEU:HA	2:M:790:LEU:HD12	1.91	0.43
2:C:861:LEU:HD21	2:C:925:TYR:CE1	2.54	0.43
2:M:1086:ARG:NH1	3:N:88:TYR:CZ	2.87	0.43
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.99	0.43
2:M:21:ILE:CD1	2:M:21:ILE:H	2.30	0.43
3:N:601:ARG:CZ	3:N:613:ARG:HH21	2.31	0.43
1:L:152:PRO:HB2	1:L:155:LYS:HG3	2.01	0.43
2:M:1049:LEU:HD23	3:N:1472:ILE:HD11	2.00	0.43
2:M:958:THR:HB	9:M:2134:HOH:O	2.18	0.43
1:K:88:ARG:NH2	9:K:1273:HOH:O	2.51	0.43
5:P:309:LYS:HG3	9:P:5453:HOH:O	2.19	0.43
5:P:324:GLU:O	5:P:325:LYS:HD3	2.18	0.43
5:P:83:GLN:O	5:P:86:HIS:HB2	2.19	0.43
2:C:679:PHE:C	3:D:943:THR:HG22	2.38	0.43
2:C:607:ASP:C	2:C:609:ASN:N	2.71	0.43
3:N:549:ASN:HD22	3:N:549:ASN:HA	1.65	0.43
2:C:1:MET:N	9:C:9648:HOH:O	2.52	0.43
3:N:380:GLU:O	3:N:382:GLU:N	2.49	0.43
5:P:411:HIS:HB3	9:P:2127:HOH:O	2.17	0.43
4:E:68:LEU:HA	4:E:73:LEU:HD12	2.00	0.43
2:M:750:LYS:HG2	9:M:2076:HOH:O	2.18	0.43
2:C:279:GLU:HG3	2:C:493:ARG:NH2	2.33	0.43
3:N:227:LEU:HA	9:P:1787:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:151:LEU:O	5:F:155:THR:HB	2.19	0.43
5:F:155:THR:HG22	5:F:156:VAL:N	2.33	0.43
2:C:1083:GLU:OE1	2:C:1083:GLU:HA	2.17	0.43
2:M:160:ALA:CB	2:M:174:LEU:HD12	2.49	0.43
2:C:549:PHE:HE2	2:C:887:GLU:HA	1.83	0.43
2:M:397:GLU:C	2:M:399:ASN:N	2.73	0.43
3:N:804:LEU:HD12	3:N:806:PHE:H	1.84	0.43
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.47	0.43
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.48	0.43
3:N:1442:ASN:C	3:N:1442:ASN:HD22	2.22	0.43
5:P:93:LEU:HD21	5:P:102:LEU:HD11	2.00	0.43
2:M:172:ILE:HG12	2:M:186:VAL:CG1	2.49	0.43
3:N:991:GLN:O	3:N:994:GLN:HB3	2.18	0.43
1:A:100:LEU:HD11	9:A:9576:HOH:O	2.18	0.43
1:A:10:VAL:O	1:A:12:THR:HG23	2.18	0.43
3:D:414:ARG:HH11	3:D:414:ARG:HG3	1.82	0.43
1:B:1:MET:SD	1:B:5:LYS:HG2	2.59	0.43
5:F:100:VAL:HG21	9:F:9872:HOH:O	2.17	0.43
3:D:402:PRO:HG2	3:D:444:VAL:HG11	2.01	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
5:P:410:TYR:O	5:P:413:SER:HB2	2.19	0.43
3:D:965:GLU:O	3:D:968:ASP:HB3	2.18	0.43
2:M:93:PRO:HG3	9:M:9555:HOH:O	2.19	0.43
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.54	0.43
3:D:1378:TYR:HB2	9:D:9729:HOH:O	2.19	0.43
2:M:166:PRO:HD2	9:M:9325:HOH:O	2.18	0.43
2:M:288:ARG:HG3	9:M:9500:HOH:O	2.18	0.43
3:D:213:VAL:HG22	9:D:2107:HOH:O	2.17	0.43
3:N:122:GLU:HB2	9:N:9548:HOH:O	2.17	0.43
2:M:308:ARG:HD3	9:M:9332:HOH:O	2.19	0.43
4:O:54:LEU:HD11	9:O:4249:HOH:O	2.18	0.43
2:C:588:VAL:HG21	2:C:664:GLY:O	2.19	0.43
2:M:1020:PRO:HG3	3:N:624:ASP:OD1	2.19	0.43
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.84	0.43
3:D:658:LEU:O	3:D:661:MET:HB2	2.19	0.43
3:D:796:ARG:HD3	3:D:862:ASP:HA	2.00	0.43
1:K:25:LEU:HD12	9:L:2122:HOH:O	2.19	0.43
3:D:601:ARG:NH2	3:D:613:ARG:HE	2.17	0.43
3:N:821:VAL:HB	9:N:9577:HOH:O	2.17	0.43
3:N:402:PRO:HG2	3:N:444:VAL:HG11	2.01	0.43
1:L:70:GLY:HA3	9:L:1193:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.00	0.43
9:N:2509:HOH:O	5:P:94:LEU:HD11	2.18	0.43
1:K:43:ILE:HD11	1:L:35:THR:HG21	2.01	0.43
2:M:625:LEU:O	2:M:627:ARG:N	2.52	0.43
3:N:601:ARG:NH1	3:N:605:ASP:HB3	2.33	0.43
2:C:1002:GLU:HG3	3:D:744:GLN:NE2	2.33	0.43
3:N:107:ASP:O	3:N:108:VAL:C	2.57	0.43
5:F:185:GLN:HB3	9:F:9576:HOH:O	2.18	0.43
2:M:204:GLN:HG3	9:M:2070:HOH:O	2.19	0.43
3:N:710:ARG:NH1	9:N:9333:HOH:O	2.46	0.43
3:N:1412:LYS:HD3	9:N:2853:HOH:O	2.19	0.43
3:D:30:GLU:HB3	3:D:40:GLU:CB	2.49	0.43
2:M:813:VAL:HG23	9:M:9381:HOH:O	2.19	0.43
3:D:138:LYS:NZ	9:D:2617:HOH:O	2.52	0.43
3:D:62:LYS:HA	9:D:2796:HOH:O	2.19	0.43
3:D:401:TYR:N	3:D:402:PRO:HD3	2.34	0.43
3:N:1287:GLU:N	9:N:9657:HOH:O	2.52	0.43
2:M:855:VAL:CG2	2:M:866:PRO:HG2	2.49	0.43
4:E:59:ASN:N	9:E:9558:HOH:O	2.52	0.43
1:B:179:PHE:HB3	1:B:197:LEU:HB3	2.01	0.43
1:L:128:HIS:NE2	1:L:131:THR:HG23	2.34	0.43
3:N:1098:LEU:N	3:N:1098:LEU:HD12	2.34	0.43
2:C:884:GLN:HG3	2:C:885:ILE:HD13	2.01	0.43
3:D:13:ALA:HB1	3:D:18:ILE:HD11	2.01	0.42
2:M:918:LEU:HD23	2:M:968:LEU:C	2.39	0.42
2:M:918:LEU:HD23	2:M:968:LEU:CA	2.49	0.42
2:M:546:LEU:HA	2:M:581:THR:HG1	1.84	0.42
3:D:423:ASP:HA	9:D:2049:HOH:O	2.18	0.42
3:D:1211:MET:HB3	3:D:1213:ARG:NE	2.33	0.42
3:D:424:GLY:N	3:D:437:VAL:HG23	2.34	0.42
3:N:567:ILE:C	3:N:571:LYS:HE2	2.39	0.42
2:M:427:VAL:HG23	9:M:2524:HOH:O	2.19	0.42
2:C:945:ARG:HH11	2:C:945:ARG:CB	2.20	0.42
2:M:148:PHE:HA	9:M:9475:HOH:O	2.19	0.42
1:K:34:VAL:HG22	1:K:181:VAL:HG21	2.00	0.42
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.92	0.42
3:D:1333:HIS:N	9:D:9823:HOH:O	2.52	0.42
3:N:834:THR:HA	3:N:838:ARG:NH2	2.35	0.42
5:F:326:ASP:O	5:F:328:PHE:HD1	2.01	0.42
1:L:176:ARG:NH1	3:N:884:ARG:CZ	2.82	0.42
1:A:22:GLU:HG3	9:A:9810:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:VAL:HB	2:C:281:LEU:HD21	2.01	0.42
3:D:829:VAL:O	3:D:835:SER:HB2	2.19	0.42
2:C:783:ARG:O	2:C:785:VAL:N	2.50	0.42
5:P:373:LYS:HA	5:P:378:GLY:C	2.39	0.42
3:N:400:VAL:C	3:N:402:PRO:HD3	2.38	0.42
3:N:39:PRO:HB2	9:N:9225:HOH:O	2.19	0.42
4:E:91:ARG:HD2	9:E:9580:HOH:O	2.17	0.42
3:N:1459:LEU:HG	9:N:9608:HOH:O	2.19	0.42
1:A:85:LEU:HD12	1:A:124:ASN:CB	2.49	0.42
1:A:88:ARG:HH11	1:A:90:LEU:HD23	1.83	0.42
5:P:316:SER:HB3	5:P:319:THR:OG1	2.19	0.42
2:C:404:LEU:HA	2:C:407:LYS:CE	2.49	0.42
1:K:182:GLU:N	9:K:1076:HOH:O	2.52	0.42
1:K:14:ARG:HG3	9:K:6203:HOH:O	2.18	0.42
3:D:166:GLN:HG3	9:D:2963:HOH:O	2.19	0.42
2:C:728:HIS:HA	9:C:2290:HOH:O	2.19	0.42
1:A:91:ASN:ND2	1:A:92:PRO:HD2	2.34	0.42
5:P:113:ILE:HG23	5:P:127:ILE:CB	2.49	0.42
3:D:827:ILE:HB	3:D:828:LYS:HD3	2.01	0.42
2:M:262:ALA:HB3	9:M:9600:HOH:O	2.18	0.42
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.54	0.42
3:D:965:GLU:OE1	3:D:968:ASP:HB3	2.18	0.42
2:C:703:ILE:N	9:C:9875:HOH:O	2.51	0.42
5:P:332:PHE:HD1	9:P:1466:HOH:O	2.00	0.42
3:D:1436:SER:HB3	9:D:9873:HOH:O	2.19	0.42
1:B:92:PRO:HB3	9:B:9565:HOH:O	2.19	0.42
3:N:69:GLU:HA	9:N:9383:HOH:O	2.17	0.42
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.19	0.42
3:D:520:LEU:CD1	3:D:521:PRO:HD2	2.40	0.42
2:C:308:ARG:HB2	9:C:9614:HOH:O	2.18	0.42
3:D:195:VAL:HG13	9:D:2043:HOH:O	2.18	0.42
3:D:127:LEU:HG	3:D:128:TYR:HD1	1.83	0.42
3:N:1389:LEU:O	3:N:1391:GLU:N	2.52	0.42
3:N:489:ARG:NH1	9:N:9727:HOH:O	2.51	0.42
2:M:208:ALA:HA	2:M:218:VAL:CG2	2.49	0.42
1:L:61:VAL:HG13	9:L:6647:HOH:O	2.20	0.42
5:F:111:GLU:HB3	9:F:9921:HOH:O	2.19	0.42
1:K:53:VAL:HG21	1:K:82:LEU:HB3	2.00	0.42
2:M:651:LYS:HG2	9:M:9533:HOH:O	2.19	0.42
3:D:866:VAL:O	3:D:873:LEU:HD12	2.19	0.42
3:N:738:ALA:HB2	9:N:9228:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:369:LEU:HD21	5:F:401:GLU:OE1	2.19	0.42
1:B:85:LEU:HD12	1:B:124:ASN:CB	2.49	0.42
2:C:288:ARG:HA	2:C:288:ARG:NH1	2.34	0.42
1:B:80:LEU:HG	3:D:844:ALA:CB	2.43	0.42
2:C:776:SER:HA	2:C:780:GLU:CB	2.44	0.42
3:N:206:ARG:HB2	9:N:2716:HOH:O	2.19	0.42
5:P:93:LEU:HB2	9:P:2248:HOH:O	2.19	0.42
3:N:537:THR:HA	5:P:317:LEU:HD12	2.01	0.42
1:K:39:PRO:HG3	1:L:39:PRO:HG3	2.01	0.42
1:A:142:VAL:HG23	1:A:142:VAL:O	2.18	0.42
3:N:10:ILE:O	3:N:1454:GLY:HA2	2.19	0.42
1:L:48:ILE:HD13	1:L:210:ALA:HB1	2.00	0.42
3:N:566:ILE:HG23	5:P:214:GLN:OE1	2.19	0.42
5:F:94:LEU:H	5:F:98:GLU:HB2	1.83	0.42
2:M:234:ALA:HB2	9:M:9679:HOH:O	2.19	0.42
5:P:113:ILE:HA	5:P:116:LEU:HD12	2.01	0.42
5:F:208:SER:HB2	5:F:211:ASP:OD1	2.19	0.42
2:C:679:PHE:O	3:D:943:THR:HG22	2.19	0.42
2:C:1009:SER:HB3	9:C:9882:HOH:O	2.19	0.42
2:C:614:ARG:HD3	9:C:9979:HOH:O	2.19	0.42
3:D:669:ASN:O	3:D:672:ALA:HB3	2.19	0.42
2:C:798:GLY:HA3	2:C:828:ALA:O	2.18	0.42
1:B:5:LYS:O	1:B:8:ALA:HB2	2.20	0.42
3:N:176:ASP:HA	9:N:9302:HOH:O	2.19	0.42
3:D:2:LYS:HB3	9:D:2307:HOH:O	2.17	0.42
1:A:128:HIS:O	1:A:129:ILE:HD13	2.19	0.42
3:D:101:HIS:HD2	3:D:582:LEU:HD13	1.84	0.42
1:L:128:HIS:HB2	9:L:7862:HOH:O	2.18	0.42
3:N:1094:LEU:HD23	3:N:1230:GLY:HA2	2.01	0.42
3:N:79:GLU:HG2	9:N:2381:HOH:O	2.18	0.42
3:D:1486:VAL:HG22	9:D:9984:HOH:O	2.19	0.42
3:D:1428:ALA:O	3:D:1430:SER:N	2.52	0.42
2:M:915:LYS:HB3	9:M:9311:HOH:O	2.19	0.42
3:N:424:GLY:CA	3:N:436:GLU:HA	2.37	0.42
2:M:139:GLN:HA	2:M:411:SER:O	2.19	0.42
2:M:325:ILE:HG13	2:M:325:ILE:H	1.60	0.42
2:C:971:LYS:HG2	2:C:988:VAL:HG12	2.02	0.42
3:N:119:SER:N	3:N:123:LEU:HB2	2.34	0.42
3:D:890:VAL:HG11	3:D:922:LEU:HD13	2.01	0.42
2:C:77:PRO:HD2	2:C:91:GLN:O	2.19	0.42
3:D:190:GLU:HG3	3:D:210:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:397:ILE:HD13	9:F:9936:HOH:O	2.19	0.42
5:P:335:ASP:CG	5:P:338:LEU:HD12	2.39	0.42
4:E:32:ARG:C	4:E:34:GLY:H	2.23	0.42
2:C:734:LEU:HD12	9:C:9587:HOH:O	2.17	0.42
2:C:737:LEU:HD22	2:C:741:GLY:O	2.19	0.42
1:K:221:HIS:ND1	1:K:224:TYR:HE2	2.15	0.42
5:F:416:ARG:HB3	9:F:9972:HOH:O	2.19	0.42
3:D:613:ARG:HH11	3:D:613:ARG:HG3	1.83	0.42
3:N:813:LEU:HD11	9:N:9724:HOH:O	2.19	0.42
3:N:669:ASN:O	3:N:672:ALA:HB3	2.18	0.42
1:B:133:GLU:HG2	9:B:9650:HOH:O	2.19	0.42
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.50	0.42
2:C:890:LEU:HG	2:C:901:TYR:CD1	2.53	0.42
1:A:133:GLU:HB3	9:A:9624:HOH:O	2.18	0.42
3:N:58:CYS:SG	3:N:59:ALA:N	2.92	0.42
5:P:207:LEU:HD11	5:P:251:ILE:HA	2.01	0.42
1:K:209:GLU:O	1:K:213:GLN:HG3	2.19	0.42
2:C:384:GLU:HA	2:C:388:ARG:NH2	2.34	0.42
3:D:898:GLU:HA	9:D:2154:HOH:O	2.19	0.42
3:N:988:ARG:HD2	3:N:992:ILE:HD12	2.00	0.42
2:M:672:VAL:HG23	2:M:868:ASP:OD2	2.19	0.42
5:P:403:LYS:HA	5:P:403:LYS:HD3	1.84	0.42
2:C:72:ARG:HD3	9:C:2792:HOH:O	2.18	0.42
3:D:1223:ILE:CD1	3:D:1462:LEU:HD12	2.50	0.42
5:F:159:ILE:O	5:F:163:LEU:HG	2.20	0.42
2:C:877:PRO:HD3	3:D:949:ILE:HD11	1.99	0.42
2:M:47:ALA:O	2:M:50:GLU:HB2	2.18	0.42
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.85	0.42
3:D:50:PHE:CB	3:D:522:PRO:HG2	2.50	0.42
3:D:212:ARG:HD2	3:D:445:ARG:NH1	2.34	0.42
2:M:321:GLU:HA	9:M:9664:HOH:O	2.20	0.42
2:M:209:ARG:O	2:M:213:ALA:HB2	2.19	0.42
3:N:139:GLY:HA3	3:N:452:ILE:HD12	2.01	0.42
3:D:583:ASP:HA	3:D:602:SER:CB	2.49	0.42
3:N:850:LEU:O	3:N:853:VAL:HB	2.19	0.42
3:N:703:ASN:HA	3:N:703:ASN:HD22	1.73	0.42
3:D:799:LYS:HD3	9:D:2211:HOH:O	2.18	0.42
3:N:167:GLU:HG2	9:N:2697:HOH:O	2.20	0.42
3:N:1442:ASN:ND2	3:N:1442:ASN:H	2.17	0.42
1:B:44:LEU:HD23	1:B:48:ILE:CD1	2.45	0.42
1:A:72:LYS:HA	9:C:9832:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:GLU:HB3	2:C:912:PRO:HD3	2.01	0.42
2:C:793:PRO:HB2	9:C:9660:HOH:O	2.18	0.42
3:D:1490:LYS:HB3	9:D:2818:HOH:O	2.19	0.42
2:M:299:LYS:HE2	9:M:9257:HOH:O	2.20	0.42
2:M:948:GLU:HB2	2:M:955:PRO:HG3	2.01	0.42
3:N:476:GLU:HA	9:N:9645:HOH:O	2.19	0.42
3:N:47:GLU:HA	3:N:51:GLY:O	2.19	0.42
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	2.02	0.42
3:D:105:VAL:HG12	3:D:106:LYS:HE3	2.01	0.42
2:M:617:ASP:HB2	9:M:9795:HOH:O	2.18	0.42
1:L:34:VAL:HG22	1:L:181:VAL:HG21	2.01	0.42
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	2.01	0.42
3:D:517:VAL:HG12	3:D:518:PRO:O	2.20	0.42
3:N:179:VAL:HG23	9:N:2700:HOH:O	2.18	0.42
2:M:418:LEU:HB3	9:M:9342:HOH:O	2.19	0.42
1:A:34:VAL:HG21	2:C:939:ARG:HD2	2.01	0.42
3:D:679:ARG:HH12	3:D:681:ARG:CD	2.24	0.42
5:F:276:ARG:HG2	9:F:9570:HOH:O	2.18	0.42
3:D:1138:ALA:O	3:D:1141:GLU:HB2	2.20	0.42
2:C:557:ARG:CZ	2:C:560:MET:SD	3.07	0.42
3:N:858:VAL:HG12	3:N:859:ASP:O	2.19	0.42
4:E:54:LEU:HG	4:E:58:PRO:CD	2.48	0.42
2:M:15:LEU:HB2	2:M:586:ARG:NH2	2.33	0.42
2:M:395:LYS:CG	2:M:397:GLU:HG2	2.47	0.42
2:C:473:ARG:NE	2:C:531:PHE:HE1	2.11	0.42
3:D:162:ARG:HB2	3:D:162:ARG:NH1	2.34	0.42
3:N:1331:ASP:OD1	3:N:1333:HIS:HB2	2.20	0.42
2:M:713:ARG:NH1	2:M:713:ARG:HG2	2.34	0.42
3:D:656:PHE:HB3	3:D:694:VAL:HG11	2.01	0.42
2:C:606:VAL:HG22	2:C:645:VAL:HG13	2.01	0.42
1:A:227:ASN:ND2	1:A:227:ASN:N	2.61	0.42
2:C:478:VAL:CG1	2:C:506:ASN:HB3	2.49	0.42
5:F:187:LEU:HD23	5:F:191:ASN:ND2	2.35	0.42
2:C:578:VAL:CG2	2:C:579:VAL:HG12	2.49	0.42
3:N:36:THR:C	3:N:38:LYS:N	2.72	0.42
2:C:678:PRO:O	3:D:943:THR:HA	2.19	0.42
3:N:1197:ARG:HD2	3:N:1396:GLU:HB2	2.02	0.42
3:D:1087:ARG:HH21	3:D:1238:MET:HB2	1.84	0.42
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.55	0.42
2:M:928:LYS:HA	9:M:9477:HOH:O	2.20	0.42
3:D:15:PRO:HG3	9:D:9724:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:30:LEU:HD11	9:M:9879:HOH:O	2.19	0.42
9:M:9885:HOH:O	3:N:628:ARG:HD3	2.19	0.42
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	2.01	0.42
3:D:421:LEU:HD21	9:D:9882:HOH:O	2.19	0.42
5:P:358:LEU:O	5:P:358:LEU:HD23	2.19	0.42
2:M:71:TYR:HD2	2:M:71:TYR:H	1.67	0.42
3:D:205:TYR:CE2	3:D:393:ILE:HG12	2.55	0.42
3:N:426:LYS:HB3	3:N:426:LYS:HE2	1.90	0.42
2:C:151:ASP:HB2	2:C:157:ARG:O	2.19	0.42
3:D:112:ILE:HD11	3:D:116:LEU:HD12	2.00	0.42
4:E:10:PHE:O	4:E:13:VAL:HG22	2.20	0.42
2:C:601:GLY:O	2:C:648:ARG:HA	2.19	0.42
5:F:164:LYS:HA	5:F:171:LYS:HZ2	1.81	0.42
2:M:685:GLU:HG3	3:N:783:ARG:HD2	2.01	0.42
2:M:651:LYS:HA	9:M:2442:HOH:O	2.19	0.42
3:D:819:GLY:HA3	9:D:3219:HOH:O	2.18	0.42
2:C:530:GLU:O	2:C:531:PHE:HD1	2.03	0.42
2:M:1043:TYR:CE2	3:N:763:MET:HG3	2.54	0.42
3:N:699:VAL:HB	3:N:716:PHE:O	2.20	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.87	0.42
1:B:48:ILE:HD13	1:B:210:ALA:HB1	2.02	0.42
5:F:216:GLY:O	5:F:243:ILE:HG12	2.19	0.42
5:P:201:LYS:HD2	9:P:8888:HOH:O	2.19	0.42
3:N:546:ARG:O	3:N:550:ARG:HG2	2.20	0.42
2:M:299:LYS:HG3	9:M:9257:HOH:O	2.18	0.42
3:D:1193:THR:N	9:D:9658:HOH:O	2.52	0.42
2:M:1105:LYS:HB2	2:M:1107:ASN:ND2	2.35	0.42
2:C:525:SER:HA	9:C:9711:HOH:O	2.19	0.42
2:C:441:VAL:HG23	9:C:2264:HOH:O	2.20	0.42
2:C:115:LEU:HG	2:C:115:LEU:H	1.70	0.42
3:N:231:VAL:HA	3:N:378:ILE:CB	2.50	0.42
1:B:122:ILE:HD12	9:B:9579:HOH:O	2.18	0.42
3:D:48:ARG:HA	9:D:2217:HOH:O	2.19	0.42
2:M:435:TYR:CE1	2:M:539:VAL:HG22	2.54	0.42
3:D:65:ARG:HG3	3:D:66:GLN:H	1.84	0.42
2:M:165:LEU:HD12	2:M:166:PRO:HA	2.01	0.42
1:A:34:VAL:HG23	9:A:9562:HOH:O	2.18	0.42
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.49	0.42
3:D:205:TYR:HA	3:D:393:ILE:HD13	2.01	0.42
2:C:841:ASN:C	2:C:841:ASN:ND2	2.71	0.42
3:N:480:GLU:O	3:N:484:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.54	0.42
3:N:26:VAL:HG23	9:N:9259:HOH:O	2.19	0.42
1:K:33:GLY:HA2	1:K:195:LEU:HD22	2.01	0.42
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	2.01	0.42
3:N:645:PRO:HG2	3:N:724:GLN:O	2.19	0.42
1:A:74:ASP:HB2	9:A:9794:HOH:O	2.19	0.42
2:M:724:ARG:HB2	2:M:740:GLU:CA	2.43	0.42
2:C:948:GLU:HB2	2:C:955:PRO:HG3	2.02	0.42
4:O:84:ARG:HD2	9:O:3299:HOH:O	2.19	0.42
4:E:40:LEU:HB2	4:E:45:ARG:CZ	2.49	0.42
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.49	0.42
3:N:796:ARG:HE	3:N:828:LYS:HZ3	1.68	0.42
3:N:559:ALA:O	5:P:132:ARG:NH1	2.52	0.42
3:D:729:HIS:HE1	3:D:731:LEU:HG	1.83	0.42
1:L:103:ALA:HB1	9:L:4720:HOH:O	2.20	0.42
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.53	0.42
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.54	0.42
1:K:178:ALA:HB2	2:M:864:GLY:CA	2.50	0.42
3:D:644:LEU:O	3:D:721:VAL:HG22	2.20	0.42
2:M:480:THR:HG22	2:M:481:ASP:N	2.35	0.42
2:M:292:ARG:NH2	2:M:299:LYS:HD3	2.35	0.42
2:C:744:ARG:NE	9:C:9710:HOH:O	2.50	0.42
1:B:90:LEU:CD2	1:B:91:ASN:HD22	2.33	0.42
2:C:514:VAL:HG13	9:C:9943:HOH:O	2.19	0.42
3:D:894:LYS:HB3	9:D:2360:HOH:O	2.19	0.42
3:D:1275:SER:HA	3:D:1303:TYR:CE1	2.54	0.42
2:C:572:ILE:HG13	2:C:573:ARG:N	2.34	0.42
3:D:1194:CYS:HB2	9:D:2009:HOH:O	2.19	0.42
1:B:75:VAL:O	1:B:79:ILE:HG23	2.19	0.42
5:P:149:GLU:HB2	9:P:3104:HOH:O	2.18	0.42
3:D:1250:ALA:HB3	9:D:3244:HOH:O	2.19	0.42
2:M:517:ARG:O	2:M:519:GLY:N	2.52	0.42
3:D:1389:LEU:O	3:D:1391:GLU:N	2.53	0.42
2:C:625:LEU:O	2:C:627:ARG:N	2.53	0.42
3:N:527:MET:CE	3:N:535:PHE:HB3	2.50	0.42
3:N:528:VAL:O	3:N:535:PHE:HA	2.20	0.42
2:M:46:ALA:O	2:M:50:GLU:HG3	2.20	0.42
3:N:422:ALA:H	3:N:427:VAL:CG1	2.33	0.42
2:M:939:ARG:CZ	9:M:9419:HOH:O	2.66	0.42
3:N:44:LEU:HG	9:N:9241:HOH:O	2.20	0.42
3:N:434:ARG:HB2	3:N:447:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASP:CB	9:A:9794:HOH:O	2.67	0.42
3:N:728:LEU:HD12	3:N:729:HIS:N	2.34	0.42
2:M:182:VAL:HG12	9:M:9802:HOH:O	2.19	0.42
4:E:66:LYS:HB2	4:E:66:LYS:NZ	2.35	0.42
2:M:949:LYS:HZ2	3:N:796:ARG:HH22	1.67	0.42
2:C:492:ASP:CA	2:C:518:LYS:HB3	2.47	0.42
2:M:16:PRO:HB3	2:M:460:ARG:NH1	2.35	0.42
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.35	0.42
2:M:575:GLN:HE21	2:M:671:ASN:HB2	1.85	0.42
3:D:1503:VAL:HG21	9:D:9933:HOH:O	2.20	0.42
1:A:72:LYS:N	9:A:9656:HOH:O	2.53	0.42
1:K:198:ARG:NE	9:K:1703:HOH:O	2.53	0.42
3:N:93:ILE:HG13	3:N:519:VAL:CG2	2.50	0.42
2:M:753:ASP:OD2	3:N:681:ARG:HD2	2.20	0.42
5:P:207:LEU:HD12	5:P:251:ILE:HG12	2.01	0.42
3:N:1020:LEU:HG	3:N:1035:ILE:HD12	2.00	0.42
3:D:1300:SER:HB3	9:D:9737:HOH:O	2.20	0.42
2:C:853:LEU:HB2	2:C:858:MET:HE3	2.01	0.42
3:D:1156:LEU:HD11	3:D:1177:ALA:HA	2.02	0.42
2:C:599:GLU:HB2	9:C:2285:HOH:O	2.20	0.42
2:C:1082:PRO:HA	9:C:9720:HOH:O	2.20	0.42
2:C:627:ARG:CG	2:C:628:PHE:H	2.33	0.42
5:P:371:LEU:HD12	9:P:1495:HOH:O	2.19	0.42
3:D:525:ARG:N	3:D:526:PRO:HD3	2.35	0.42
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.50	0.42
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.75	0.42
2:M:649:VAL:HG12	2:M:650:ARG:HH21	1.85	0.42
2:M:207:LEU:HD13	2:M:221:LEU:CD1	2.50	0.42
2:C:418:LEU:HD12	9:C:2110:HOH:O	2.20	0.42
3:N:838:ARG:HH11	3:N:863:VAL:HB	1.85	0.42
3:N:860:LEU:O	3:N:876:SER:OG	2.37	0.42
3:N:751:LEU:HD13	9:N:9380:HOH:O	2.19	0.42
2:C:1014:SER:N	9:C:2050:HOH:O	2.52	0.42
4:E:54:LEU:HA	4:E:58:PRO:HG2	2.02	0.42
2:C:906:PHE:N	9:C:9623:HOH:O	2.53	0.42
3:D:1166:LEU:HD23	3:D:1166:LEU:N	2.30	0.42
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.55	0.42
5:F:421:PHE:C	5:F:423:ASP:N	2.72	0.42
3:D:601:ARG:HH22	3:D:613:ARG:HB2	1.84	0.42
2:C:471:TYR:HB3	2:C:531:PHE:CD2	2.55	0.42
4:E:41:GLU:HA	4:E:45:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:9896:HOH:O	5:P:373:LYS:HD2	2.19	0.42
1:A:177:VAL:HG12	1:A:178:ALA:N	2.35	0.42
1:A:177:VAL:O	2:C:864:GLY:CA	2.68	0.42
3:D:43:GLY:N	9:D:9655:HOH:O	2.53	0.42
2:M:172:ILE:HG13	9:M:9595:HOH:O	2.20	0.42
3:N:1033:GLN:O	3:N:1037:GLN:HG3	2.20	0.42
3:N:438:ASP:OD2	3:N:440:VAL:HB	2.19	0.42
2:M:929:ARG:HD3	9:M:9262:HOH:O	2.18	0.42
3:N:660:LYS:O	3:N:663:GLU:HB2	2.20	0.42
2:C:714:ASP:HB2	2:C:818:GLY:O	2.20	0.42
3:D:1031:ASN:HB3	3:D:1034:GLN:CD	2.40	0.42
2:M:913:GLU:O	2:M:916:GLU:HB3	2.20	0.42
1:K:106:PRO:HA	1:K:132:LEU:O	2.20	0.42
5:F:248:ASN:HB2	9:F:9828:HOH:O	2.19	0.42
3:D:160:GLU:HA	9:D:2658:HOH:O	2.18	0.42
3:D:111:LYS:HD3	3:D:111:LYS:HA	1.87	0.42
3:D:1348:LEU:HD23	3:D:1375:MET:HE3	2.02	0.42
3:D:1103:HIS:HD2	3:D:1462:LEU:H	1.67	0.42
3:D:1466:VAL:HG22	3:D:1472:ILE:CD1	2.50	0.42
3:D:983:LEU:N	9:D:2242:HOH:O	2.48	0.42
5:F:151:LEU:HB2	5:F:155:THR:CB	2.50	0.42
3:N:715:ALA:HB3	3:N:764:LEU:CA	2.35	0.42
2:M:601:GLY:O	2:M:648:ARG:HA	2.20	0.42
5:P:367:MET:O	5:P:370:LYS:HG2	2.20	0.42
2:C:359:MET:HB2	9:C:2205:HOH:O	2.18	0.42
2:C:1085:PHE:CE2	3:D:1468:LEU:HA	2.54	0.42
3:N:1428:ALA:O	3:N:1430:SER:N	2.53	0.42
3:N:128:TYR:HA	3:N:128:TYR:HD2	1.64	0.42
3:D:445:ARG:HD3	9:D:2510:HOH:O	2.20	0.42
3:N:565:ILE:CD1	3:N:565:ILE:H	2.20	0.42
2:M:192:PRO:CB	2:M:195:LEU:HD13	2.44	0.42
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.20	0.42
5:P:393:THR:CG2	5:P:394:ARG:N	2.83	0.42
2:M:585:GLU:CG	2:M:586:ARG:H	2.33	0.42
3:N:1314:LYS:HG3	9:N:2352:HOH:O	2.20	0.42
5:F:196:VAL:O	5:F:200:LYS:HB2	2.19	0.42
1:L:85:LEU:HD12	1:L:124:ASN:CB	2.50	0.42
5:F:419:ARG:HG2	5:F:419:ARG:NH1	2.35	0.42
3:D:55:ASP:HA	9:D:9689:HOH:O	2.20	0.42
1:L:175:ARG:O	3:N:851:LEU:HD21	2.20	0.42
1:L:176:ARG:NH1	3:N:884:ARG:NE	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:300:ASP:C	2:M:302:VAL:H	2.22	0.42
2:C:10:ARG:HD2	2:C:10:ARG:HA	1.80	0.42
2:C:780:GLU:HG3	2:C:781:LYS:N	2.31	0.42
4:E:51:LEU:HD12	4:E:52:GLU:H	1.83	0.42
3:D:914:LEU:O	3:D:914:LEU:HD23	2.19	0.42
3:N:417:PRO:HB3	9:P:4142:HOH:O	2.20	0.42
3:N:125:GLN:HG3	9:N:9692:HOH:O	2.20	0.42
3:D:631:ILE:HG21	3:D:745:MET:CG	2.47	0.42
1:A:30:ARG:HD2	9:D:9595:HOH:O	2.20	0.42
2:C:1036:GLU:CD	2:C:1036:GLU:N	2.73	0.42
3:N:16:GLU:O	3:N:19:ARG:HB2	2.20	0.42
2:M:248:PRO:HD3	9:M:9536:HOH:O	2.18	0.42
5:P:256:ARG:HD3	5:P:260:ILE:HG22	2.02	0.42
3:D:1284:GLU:HA	3:D:1284:GLU:OE1	2.20	0.42
2:M:850:ALA:HB1	3:N:632:VAL:HG13	2.02	0.42
4:E:43:GLU:H	4:E:43:GLU:HG2	1.66	0.42
3:D:739:ASP:CG	3:D:741:ASP:OD1	2.58	0.42
3:N:1234:THR:HA	9:N:2227:HOH:O	2.19	0.42
2:C:431:HIS:O	2:C:434:HIS:HB2	2.19	0.41
5:P:287:THR:C	5:P:289:GLU:H	2.23	0.41
3:N:168:THR:HB	3:N:170:PRO:HD3	2.03	0.41
3:N:186:VAL:HG23	3:N:211:VAL:CG1	2.49	0.41
3:D:486:ARG:HH21	3:D:489:ARG:CD	2.32	0.41
2:C:110:GLU:HB3	2:C:368:THR:HG22	2.02	0.41
2:C:405:ARG:HD2	9:C:9844:HOH:O	2.19	0.41
2:M:514:VAL:HG12	2:M:515:ALA:N	2.35	0.41
2:C:130:ASN:CG	2:C:383:ARG:HH22	2.24	0.41
2:C:244:PRO:CD	2:C:245:GLY:N	2.82	0.41
1:A:217:ILE:H	1:A:217:ILE:HG13	1.70	0.41
3:N:907:GLU:CD	3:N:909:ASN:HB2	2.40	0.41
5:F:289:GLU:O	5:F:293:GLU:HG3	2.19	0.41
3:D:871:LYS:CG	3:D:873:LEU:HG	2.49	0.41
5:P:394:ARG:HA	5:P:397:ILE:CD1	2.45	0.41
4:E:48:MET:HG2	4:E:49:GLN:N	2.34	0.41
1:L:90:LEU:HB3	9:L:1485:HOH:O	2.19	0.41
4:O:87:LYS:HE2	4:O:91:ARG:NH2	2.28	0.41
5:F:363:GLU:HA	9:F:9838:HOH:O	2.20	0.41
1:K:86:VAL:HG13	1:K:86:VAL:O	2.20	0.41
3:D:434:ARG:CB	3:D:447:VAL:HG13	2.49	0.41
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.20	0.41
3:N:399:ARG:HB3	3:N:402:PRO:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HD21	2:M:542:VAL:HG11	2.01	0.41
5:P:291:ILE:CG2	5:P:304:VAL:HG21	2.49	0.41
2:M:1037:VAL:O	2:M:1041:GLU:HG3	2.20	0.41
1:A:106:PRO:HA	1:A:132:LEU:O	2.20	0.41
2:M:246:ASP:HB2	9:M:9223:HOH:O	2.19	0.41
2:M:897:LEU:HB3	2:M:899:GLN:CG	2.50	0.41
5:P:80:PRO:O	5:P:83:GLN:HB2	2.20	0.41
2:C:872:ASN:HA	2:C:873:PRO:HD3	1.89	0.41
3:N:656:PHE:HB3	3:N:694:VAL:HG11	2.01	0.41
2:C:264:PRO:HB2	9:C:9902:HOH:O	2.20	0.41
1:L:5:LYS:O	1:L:8:ALA:HB2	2.20	0.41
2:C:84:ARG:HH12	2:C:128:ILE:CD1	2.33	0.41
3:N:112:ILE:HD11	3:N:124:GLU:CG	2.50	0.41
3:N:30:GLU:HB3	3:N:40:GLU:CG	2.50	0.41
3:D:1274:ILE:H	3:D:1274:ILE:HG13	1.58	0.41
3:N:1041:LEU:HD12	3:N:1058:ARG:HA	2.02	0.41
5:F:104:ARG:NH2	9:F:9811:HOH:O	2.52	0.41
3:D:792:ILE:O	3:D:878:GLY:HA3	2.20	0.41
5:P:253:ASP:HB3	5:P:259:ARG:HH21	1.85	0.41
3:D:33:ASN:HA	9:F:9722:HOH:O	2.19	0.41
3:N:213:VAL:HG13	9:N:2214:HOH:O	2.19	0.41
5:P:367:MET:HA	5:P:370:LYS:CD	2.49	0.41
3:N:9:ARG:NH1	3:N:9:ARG:HG2	2.35	0.41
2:C:1087:VAL:O	2:C:1091:GLU:HG3	2.20	0.41
2:M:143:SER:CB	2:M:276:LYS:HE2	2.49	0.41
3:D:168:THR:C	3:D:170:PRO:HD3	2.41	0.41
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.50	0.41
3:N:1146:GLY:N	9:N:2585:HOH:O	2.53	0.41
1:B:132:LEU:HD21	1:B:138:LEU:HB2	2.02	0.41
3:N:161:LEU:C	3:N:449:SER:HB2	2.41	0.41
3:D:1335:LEU:HD21	9:D:9849:HOH:O	2.20	0.41
2:C:1016:ILE:HD11	5:F:330:GLY:CA	2.50	0.41
9:D:2988:HOH:O	4:E:58:PRO:HG3	2.19	0.41
2:C:887:GLU:HG3	9:C:9563:HOH:O	2.20	0.41
3:D:794:GLN:NE2	3:D:795:VAL:N	2.68	0.41
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.35	0.41
5:F:366:ALA:HB3	9:F:9838:HOH:O	2.19	0.41
3:N:1301:LYS:HD3	9:N:2604:HOH:O	2.18	0.41
3:N:209:ARG:NH1	3:N:397:LYS:HG3	2.35	0.41
1:B:41:ARG:HH11	1:B:41:ARG:HG3	1.85	0.41
2:M:757:GLY:HA2	2:M:789:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:524:VAL:HG22	2:M:528:GLU:HB2	2.01	0.41
2:C:1067:TYR:CB	5:F:341:PRO:HB3	2.50	0.41
5:F:402:ASN:HB3	5:F:406:ARG:NH1	2.35	0.41
3:N:793:THR:HB	3:N:879:ARG:HD2	2.02	0.41
3:D:996:TRP:CE3	3:D:996:TRP:HA	2.54	0.41
3:N:659:LYS:O	3:N:663:GLU:HG2	2.20	0.41
3:D:414:ARG:HB3	9:D:2090:HOH:O	2.20	0.41
1:B:8:ALA:HB2	9:B:9765:HOH:O	2.20	0.41
2:C:384:GLU:HG3	2:C:388:ARG:HB2	2.02	0.41
3:N:1307:LYS:HB2	3:N:1307:LYS:NZ	2.35	0.41
2:M:464:LEU:HD13	9:M:9893:HOH:O	2.20	0.41
1:A:3:ASP:HB3	1:A:4:SER:H	1.54	0.41
5:P:387:GLY:HA2	9:P:8096:HOH:O	2.19	0.41
3:D:47:GLU:HA	3:D:51:GLY:O	2.20	0.41
5:P:75:ILE:HG22	9:P:6479:HOH:O	2.18	0.41
1:B:55:SER:HB2	1:B:158:ILE:HB	2.02	0.41
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.20	0.41
2:M:854:PRO:C	2:M:856:GLU:N	2.73	0.41
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.19	0.41
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.41
3:N:131:LYS:HB3	3:N:131:LYS:HZ3	1.85	0.41
3:N:567:ILE:O	3:N:571:LYS:HG3	2.20	0.41
3:N:427:VAL:HG21	3:N:435:VAL:HB	2.03	0.41
2:M:514:VAL:HG11	2:M:516:ARG:CZ	2.50	0.41
2:M:497:ALA:HB3	2:M:532:MET:HG3	2.02	0.41
2:C:73:LEU:HD23	2:C:118:ILE:HD11	2.01	0.41
3:N:829:VAL:HA	9:N:9736:HOH:O	2.19	0.41
3:N:116:LEU:CB	3:N:118:LEU:HD13	2.44	0.41
2:M:230:ARG:CZ	2:M:237:ARG:HH22	2.32	0.41
2:M:241:LEU:HG	9:M:9694:HOH:O	2.21	0.41
3:N:907:GLU:OE2	3:N:909:ASN:HB2	2.21	0.41
2:C:690:ILE:HG12	2:C:849:VAL:HG13	2.01	0.41
2:M:1115:LEU:CD2	3:N:85:VAL:HG22	2.50	0.41
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.53	0.41
2:C:1016:ILE:CD1	5:F:317:LEU:HD21	2.43	0.41
5:F:317:LEU:O	5:F:329:TYR:HB3	2.21	0.41
3:N:1312:LEU:HD23	9:N:2549:HOH:O	2.20	0.41
3:N:1467:ILE:HD13	9:N:9712:HOH:O	2.20	0.41
3:N:1278:ASP:OD1	3:N:1321:ALA:HB2	2.20	0.41
2:M:460:ARG:HG3	2:M:460:ARG:HH11	1.85	0.41
3:N:598:ARG:HA	3:N:599:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:516:ARG:HB3	9:C:9652:HOH:O	2.19	0.41
2:M:1035:MET:HA	2:M:1038:TRP:CE3	2.55	0.41
3:D:644:LEU:CG	3:D:718:PRO:HB3	2.50	0.41
3:D:381:ALA:HA	9:D:2848:HOH:O	2.19	0.41
5:P:350:LEU:CD1	5:P:422:LEU:HD13	2.50	0.41
2:M:928:LYS:HE2	9:M:9477:HOH:O	2.20	0.41
2:C:707:ARG:HD2	2:C:824:ARG:HD3	2.01	0.41
2:C:249:LYS:HA	9:C:2727:HOH:O	2.19	0.41
5:F:301:ALA:HB2	9:F:2002:HOH:O	2.19	0.41
2:M:137:VAL:HG13	2:M:409:ARG:O	2.20	0.41
5:P:313:GLU:OE1	5:P:313:GLU:HA	2.20	0.41
2:M:366:SER:HB3	9:M:2384:HOH:O	2.20	0.41
2:C:328:LEU:HD22	2:C:433:THR:C	2.41	0.41
2:M:859:PRO:HB2	2:M:867:VAL:CG2	2.51	0.41
3:D:1209:LEU:HD23	3:D:1216:SER:H	1.85	0.41
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.20	0.41
2:M:145:GLY:H	2:M:163:ILE:HG23	1.85	0.41
2:C:988:VAL:HG13	9:C:9757:HOH:O	2.21	0.41
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.88	0.41
2:M:130:ASN:N	9:M:9614:HOH:O	2.52	0.41
2:M:205:GLU:HG3	2:M:206:THR:N	2.36	0.41
2:M:205:GLU:HG3	9:M:9651:HOH:O	2.20	0.41
2:M:207:LEU:HD13	2:M:221:LEU:HD11	2.01	0.41
3:N:637:LEU:HD11	3:N:642:CYS:HA	2.02	0.41
2:M:1047:HIS:O	2:M:1051:GLU:HG3	2.20	0.41
4:E:48:MET:N	4:E:54:LEU:HB2	2.34	0.41
1:K:2:LEU:HA	1:K:6:LEU:CD2	2.50	0.41
2:C:274:ARG:O	2:C:278:GLU:HG3	2.20	0.41
5:P:94:LEU:HD12	5:P:97:GLU:H	1.83	0.41
1:L:220:GLU:HA	1:L:223:THR:HG23	2.02	0.41
2:M:697:ARG:O	2:M:699:PHE:N	2.48	0.41
2:C:121:MET:HA	2:C:127:PHE:CE2	2.56	0.41
2:C:47:ALA:O	2:C:50:GLU:HB3	2.20	0.41
1:B:110:LYS:HG3	9:B:9637:HOH:O	2.20	0.41
1:B:108:GLU:HB3	1:B:128:HIS:HE1	1.86	0.41
1:B:89:PHE:HD2	1:B:146:ARG:HH21	1.69	0.41
3:N:1111:ASP:HB2	3:N:1203:LYS:HD2	2.03	0.41
2:C:455:LEU:HD22	2:C:459:ALA:HB1	2.02	0.41
2:C:193:LEU:HA	2:C:196:LEU:HD12	2.02	0.41
2:C:19:THR:HG22	2:C:19:THR:O	2.20	0.41
3:D:1110:ALA:O	3:D:1112:CYS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG21	1:B:82:LEU:HB3	2.03	0.41
9:K:5576:HOH:O	1:L:11:PHE:HB3	2.20	0.41
9:N:2944:HOH:O	5:P:92:PRO:HG2	2.20	0.41
3:D:1381:VAL:HG23	3:D:1391:GLU:HB2	2.01	0.41
2:M:1092:LEU:CD1	2:M:1099:VAL:HG21	2.45	0.41
3:N:521:PRO:HB3	9:N:9625:HOH:O	2.20	0.41
3:N:520:LEU:O	3:N:525:ARG:NH1	2.54	0.41
4:O:48:MET:HG2	4:O:49:GLN:N	2.33	0.41
4:O:59:ASN:HB2	9:O:4249:HOH:O	2.19	0.41
1:K:104:GLU:HA	1:K:136:GLY:O	2.21	0.41
2:C:666:LEU:HD11	2:C:668:LEU:HG	2.01	0.41
3:D:1394:VAL:CB	3:D:1397:LYS:HD2	2.51	0.41
3:D:99:ALA:CA	3:D:575:GLN:HE22	2.29	0.41
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	2.03	0.41
3:N:704:ARG:CD	9:N:9228:HOH:O	2.69	0.41
2:M:176:VAL:HG12	2:M:178:PRO:HD3	2.03	0.41
1:A:48:ILE:HD13	1:A:210:ALA:HB1	2.03	0.41
5:F:80:PRO:O	5:F:83:GLN:HB3	2.20	0.41
1:B:151:VAL:HG12	1:B:156:HIS:ND1	2.36	0.41
1:K:71:VAL:HG13	9:K:1208:HOH:O	2.19	0.41
5:P:136:LEU:HD12	5:P:137:GLY:N	2.36	0.41
1:A:88:ARG:HD2	1:A:123:MET:CE	2.50	0.41
2:C:897:LEU:HD23	2:C:899:GLN:CD	2.41	0.41
5:P:309:LYS:HA	5:P:312:GLN:OE1	2.20	0.41
3:N:82:LYS:O	3:N:84:ILE:N	2.54	0.41
1:K:184:THR:HG23	1:K:192:LEU:HB2	2.02	0.41
2:M:926:PHE:O	2:M:930:LYS:HG3	2.21	0.41
2:M:927:GLY:HA2	2:M:930:LYS:HZ3	1.83	0.41
2:M:246:ASP:HA	2:M:247:PRO:HD3	1.97	0.41
2:C:807:ARG:HD2	9:C:2016:HOH:O	2.20	0.41
3:N:1110:ALA:O	3:N:1112:CYS:N	2.53	0.41
2:C:1095:LEU:HD12	3:D:603:LEU:HD13	2.03	0.41
2:C:684:PHE:CG	2:C:685:GLU:N	2.86	0.41
3:N:1353:GLN:NE2	3:N:1365:ASP:OD2	2.53	0.41
3:D:1164:ARG:HG2	9:D:2063:HOH:O	2.20	0.41
2:M:764:GLU:HG2	9:M:9355:HOH:O	2.21	0.41
2:M:76:PRO:HB2	9:M:9838:HOH:O	2.19	0.41
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.35	0.41
3:N:191:LEU:HD22	3:N:195:VAL:HG21	2.02	0.41
2:M:858:MET:HB2	2:M:859:PRO:HD2	2.01	0.41
5:F:130:VAL:HG21	5:F:159:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:287:GLY:O	2:M:288:ARG:C	2.58	0.41
3:D:205:TYR:OH	3:D:391:ALA:HB1	2.19	0.41
3:D:1487:VAL:HG12	3:D:1488:ASP:N	2.35	0.41
5:F:288:TYR:HE2	5:F:305:GLU:HA	1.86	0.41
2:C:118:ILE:HG12	2:C:118:ILE:O	2.19	0.41
2:M:199:VAL:HG21	2:M:238:LEU:HD12	2.02	0.41
2:M:696:LYS:HA	9:M:9428:HOH:O	2.19	0.41
2:C:332:ARG:CZ	9:C:9819:HOH:O	2.69	0.41
3:D:567:ILE:O	3:D:571:LYS:HG3	2.20	0.41
3:N:860:LEU:O	3:N:877:PRO:HD2	2.20	0.41
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.20	0.41
5:F:419:ARG:O	5:F:421:PHE:N	2.53	0.41
4:E:35:PHE:N	9:E:9641:HOH:O	2.52	0.41
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.02	0.41
5:F:125:ASP:N	9:F:9847:HOH:O	2.54	0.41
2:C:172:ILE:HA	2:C:185:LYS:O	2.20	0.41
2:C:172:ILE:HG23	2:C:184:MET:CE	2.51	0.41
9:M:9803:HOH:O	3:N:1470:ARG:HA	2.21	0.41
2:C:756:VAL:HG11	2:C:823:VAL:HG21	2.02	0.41
1:K:180:GLN:NE2	9:K:1619:HOH:O	2.52	0.41
1:B:178:ALA:HB1	1:B:198:ARG:NH2	2.35	0.41
2:C:897:LEU:HD11	2:C:920:GLN:CG	2.49	0.41
3:D:899:LEU:HD13	3:D:900:ILE:HG23	2.02	0.41
5:F:406:ARG:O	5:F:409:LYS:HG2	2.20	0.41
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.35	0.41
2:C:942:GLU:HA	9:C:9752:HOH:O	2.19	0.41
2:C:279:GLU:OE2	2:C:489:THR:HG21	2.20	0.41
2:M:842:ARG:HD2	9:M:9367:HOH:O	2.21	0.41
3:N:1483:PHE:N	3:N:1483:PHE:CD1	2.89	0.41
2:C:701:THR:HG22	2:C:832:LYS:HG2	2.02	0.41
1:A:69:PRO:O	1:A:71:VAL:HG23	2.21	0.41
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.41
2:M:896:PHE:CD2	2:M:925:TYR:HB2	2.55	0.41
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.55	0.41
1:L:102:LYS:HB2	1:L:139:ASN:OD1	2.21	0.41
3:D:1263:PHE:HD2	3:D:1424:VAL:HG21	1.85	0.41
3:N:183:GLU:OE2	3:N:216:VAL:HG13	2.19	0.41
3:N:170:PRO:O	3:N:391:ALA:HB3	2.21	0.41
3:D:421:LEU:N	3:D:421:LEU:HD23	2.36	0.41
3:D:711:LEU:C	3:D:713:ILE:N	2.74	0.41
2:M:950:LEU:HB3	2:M:952:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:GLU:HA	9:C:9874:HOH:O	2.20	0.41
3:D:191:LEU:HD22	3:D:195:VAL:HG21	2.03	0.41
9:N:9507:HOH:O	5:P:134:LYS:HA	2.20	0.41
2:M:9:ILE:HG13	2:M:9:ILE:O	2.20	0.41
3:D:890:VAL:HG22	3:D:926:LYS:HG2	2.02	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
3:N:81:THR:HB	3:N:85:VAL:HG23	2.02	0.41
2:C:648:ARG:HB3	9:C:9827:HOH:O	2.21	0.41
3:N:795:VAL:HA	3:N:861:GLN:O	2.20	0.41
2:M:1063:ARG:HG3	5:P:341:PRO:HG3	2.02	0.41
2:C:1016:ILE:HD11	5:F:330:GLY:HA2	2.03	0.41
1:L:117:VAL:HG12	9:L:3068:HOH:O	2.21	0.41
5:F:131:VAL:HG22	5:F:178:ARG:HD3	2.03	0.41
3:D:991:GLN:O	3:D:994:GLN:HB3	2.20	0.41
1:L:136:GLY:HA3	9:L:2881:HOH:O	2.19	0.41
2:C:200:LEU:HD13	2:C:300:ASP:OD1	2.20	0.41
3:D:27:GLU:O	3:D:28:LYS:HG2	2.21	0.41
3:D:684:LYS:HA	9:D:2441:HOH:O	2.19	0.41
1:K:48:ILE:CG2	1:K:173:PRO:HD2	2.49	0.41
1:L:198:ARG:HD3	9:L:1055:HOH:O	2.21	0.41
3:D:3:LYS:N	3:D:3:LYS:HD3	2.34	0.41
1:B:108:GLU:O	1:B:110:LYS:HG3	2.20	0.41
2:M:297:GLU:HB3	9:M:2030:HOH:O	2.19	0.41
2:M:420:ARG:CD	2:M:420:ARG:H	2.30	0.41
3:D:35:ARG:HA	9:D:2169:HOH:O	2.21	0.41
2:M:557:ARG:HD2	2:M:557:ARG:HA	1.95	0.41
2:C:546:LEU:HG	2:C:546:LEU:O	2.21	0.41
3:D:1359:GLN:NE2	9:D:2889:HOH:O	2.52	0.41
9:N:9844:HOH:O	5:P:92:PRO:HD3	2.21	0.41
3:D:1258:ARG:HH11	3:D:1258:ARG:HG3	1.85	0.41
2:M:915:LYS:HD2	9:M:9311:HOH:O	2.20	0.41
3:N:13:ALA:O	3:N:511:TRP:HB3	2.21	0.41
2:M:690:ILE:HG21	2:M:833:LEU:HD23	2.02	0.41
3:D:119:SER:O	3:D:121:THR:N	2.54	0.41
3:N:141:ILE:HD11	3:N:431:VAL:O	2.20	0.41
2:M:206:THR:HB	9:M:9651:HOH:O	2.20	0.41
2:C:290:LEU:H	2:C:290:LEU:CD1	2.25	0.41
5:P:155:THR:HG22	5:P:159:ILE:HD11	2.03	0.41
2:M:878:SER:HB3	8:N:9101:G4P:O2D	2.21	0.41
3:N:644:LEU:HA	3:N:645:PRO:HD3	1.98	0.41
2:C:1052:MET:CE	2:C:1056:LYS:HD3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.36	0.41
3:N:796:ARG:HD2	9:N:9384:HOH:O	2.20	0.41
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.03	0.41
2:M:462:ASP:OD1	2:M:463:GLU:N	2.54	0.41
3:N:799:LYS:HD2	9:N:2444:HOH:O	2.21	0.41
2:M:502:PRO:HD3	9:M:2363:HOH:O	2.20	0.41
2:M:958:THR:HG23	2:M:961:GLU:CG	2.51	0.41
1:B:7:LYS:HZ2	1:B:7:LYS:HB3	1.86	0.41
2:C:438:ILE:HG23	2:C:453:THR:OG1	2.20	0.41
1:A:189:ARG:HG2	9:A:9613:HOH:O	2.21	0.41
3:N:1372:VAL:HA	3:N:1375:MET:HE2	2.01	0.41
3:D:16:GLU:O	3:D:19:ARG:HB2	2.20	0.41
3:N:190:GLU:HG3	3:N:210:ARG:CZ	2.50	0.41
3:D:884:ARG:O	3:D:888:GLU:N	2.53	0.41
2:C:384:GLU:CA	2:C:388:ARG:HH21	2.34	0.41
1:A:35:THR:HG22	9:B:9638:HOH:O	2.20	0.41
3:D:1103:HIS:CG	3:D:1104:GLU:N	2.89	0.41
3:D:486:ARG:HA	3:D:489:ARG:HD3	2.03	0.41
2:C:625:LEU:C	2:C:627:ARG:HH21	2.23	0.41
2:M:166:PRO:HB2	9:M:9681:HOH:O	2.21	0.41
3:D:520:LEU:O	3:D:525:ARG:NH1	2.54	0.41
2:C:405:ARG:HH11	2:C:405:ARG:HG2	1.85	0.41
3:D:119:SER:HB2	3:D:123:LEU:CB	2.42	0.41
3:D:780:LYS:NZ	3:D:912:LYS:HE3	2.36	0.41
1:A:42:ARG:NE	1:B:35:THR:OG1	2.48	0.41
1:B:106:PRO:HD2	9:B:9677:HOH:O	2.20	0.41
5:F:276:ARG:HD2	9:F:9563:HOH:O	2.21	0.41
3:N:162:ARG:HG2	9:N:9455:HOH:O	2.20	0.41
5:F:170:HIS:HA	5:F:173:TYR:HD1	1.85	0.41
3:D:100:ALA:N	9:D:2106:HOH:O	2.53	0.41
3:D:1197:ARG:C	3:D:1199:GLY:H	2.24	0.41
3:D:761:ILE:HD11	9:E:9593:HOH:O	2.20	0.41
4:E:25:LYS:HA	4:E:28:GLN:OE1	2.21	0.41
2:C:181:VAL:HG12	2:C:182:VAL:N	2.36	0.41
5:F:320:PRO:HA	9:F:9771:HOH:O	2.20	0.41
2:M:397:GLU:N	2:M:633:GLN:OE1	2.54	0.41
3:N:737:ASN:N	9:N:9545:HOH:O	2.51	0.41
3:D:1500:LYS:HA	9:D:9806:HOH:O	2.20	0.41
4:O:87:LYS:HA	9:O:4487:HOH:O	2.20	0.41
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.56	0.41
3:N:851:LEU:HD23	3:N:851:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:889:HIS:CE1	3:D:951:ILE:H	2.28	0.41
2:M:200:LEU:HD22	2:M:300:ASP:OD1	2.20	0.41
2:M:710:ILE:HB	2:M:790:LEU:HB2	2.02	0.41
5:F:361:LEU:HB3	9:F:9838:HOH:O	2.21	0.41
3:D:162:ARG:NH1	9:D:9697:HOH:O	2.50	0.41
3:D:785:ILE:N	9:D:2202:HOH:O	2.53	0.41
3:N:416:ALA:HB3	3:N:417:PRO:HD3	2.02	0.41
1:A:178:ALA:HB2	2:C:864:GLY:N	2.34	0.41
5:P:157:GLU:O	5:P:161:GLN:HG3	2.21	0.41
3:D:527:MET:HE1	3:D:535:PHE:HB3	2.02	0.41
1:K:165:ILE:HA	1:K:166:PRO:HD3	1.95	0.41
3:N:1033:GLN:HB2	9:N:2467:HOH:O	2.21	0.41
1:B:100:LEU:HB2	1:B:115:LEU:HD21	2.03	0.41
1:A:156:HIS:CD2	1:A:157:GLY:H	2.39	0.41
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.86	0.41
2:M:204:GLN:HB2	9:M:9986:HOH:O	2.20	0.41
3:N:1379:VAL:O	3:N:1392:GLY:HA2	2.21	0.41
2:C:964:LYS:O	2:C:968:LEU:HG	2.20	0.41
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.56	0.41
5:P:115:LYS:HD2	5:P:118:GLU:OE2	2.21	0.41
3:N:1124:GLN:NE2	9:N:2426:HOH:O	2.53	0.41
2:M:916:GLU:O	2:M:919:ALA:HB3	2.21	0.41
1:B:189:ARG:HG3	9:B:9584:HOH:O	2.21	0.41
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.35	0.41
3:D:789:LEU:HD11	3:D:934:LEU:HD22	2.02	0.41
2:C:27:ARG:HG3	2:C:27:ARG:NH1	2.36	0.41
2:M:504:GLU:HB2	9:M:9322:HOH:O	2.20	0.41
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.51	0.41
5:P:276:ARG:HH11	5:P:276:ARG:HG3	1.86	0.41
2:C:493:ARG:HB2	2:C:494:TYR:CE1	2.55	0.41
2:M:850:ALA:CB	3:N:632:VAL:HG13	2.51	0.41
1:K:128:HIS:O	1:K:129:ILE:HD13	2.20	0.41
3:D:1105:ILE:HD13	9:D:9754:HOH:O	2.20	0.41
3:N:823:LEU:HD11	9:N:2306:HOH:O	2.20	0.41
2:M:61:LYS:HB2	9:M:9741:HOH:O	2.20	0.41
1:L:50:GLY:O	1:L:146:ARG:HA	2.20	0.41
2:C:784:ASP:HB2	9:C:2121:HOH:O	2.19	0.41
3:D:1123:PHE:CD1	3:D:1134:LEU:HA	2.56	0.41
5:P:88:ILE:O	5:P:92:PRO:HG3	2.21	0.41
3:D:1384:PRO:HG3	3:D:1389:LEU:CA	2.51	0.41
3:N:457:GLY:HA3	3:N:568:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:172:PRO:HB3	3:D:178:LEU:HB2	2.03	0.41
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.51	0.41
2:M:843:HIS:CD2	2:M:884:GLN:HA	2.56	0.41
5:F:288:TYR:HA	5:F:291:ILE:HG22	2.03	0.41
2:M:208:ALA:O	2:M:218:VAL:HG21	2.21	0.41
2:M:385:PHE:O	2:M:389:SER:HB3	2.21	0.41
5:P:342:VAL:O	5:P:345:ALA:HB3	2.21	0.41
4:O:54:LEU:HA	4:O:58:PRO:HG2	2.03	0.41
3:N:853:VAL:HG11	3:N:860:LEU:CD2	2.51	0.41
3:N:795:VAL:HG13	3:N:863:VAL:HG13	2.02	0.41
3:D:54:LYS:CD	3:D:55:ASP:H	2.27	0.41
3:D:785:ILE:HD12	9:D:2202:HOH:O	2.19	0.41
2:C:300:ASP:C	2:C:302:VAL:H	2.24	0.41
2:M:721:ARG:HB2	2:M:759:THR:OG1	2.21	0.41
2:M:759:THR:HB	2:M:785:VAL:CG1	2.49	0.41
3:N:1311:LEU:HD22	9:N:9440:HOH:O	2.19	0.41
3:N:1036:ARG:HD3	9:N:2161:HOH:O	2.21	0.41
1:K:18:ARG:CZ	1:K:88:ARG:HH21	2.34	0.41
1:L:10:VAL:O	1:L:12:THR:HG23	2.20	0.41
5:P:153:PRO:HG2	5:P:154:LYS:H	1.86	0.41
5:P:292:ALA:HA	5:P:299:TRP:HB3	2.03	0.41
3:D:36:THR:C	3:D:38:LYS:N	2.73	0.41
5:F:110:MET:HG2	5:F:114:LYS:HE3	2.03	0.41
3:D:235:ALA:HA	9:D:2001:HOH:O	2.20	0.41
1:A:65:PHE:CE2	2:C:830:LYS:HG3	2.56	0.41
3:D:995:LEU:HD23	9:D:2129:HOH:O	2.21	0.41
2:C:820:ARG:HH11	2:C:820:ARG:HG2	1.85	0.41
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.86	0.41
1:A:35:THR:CG2	9:B:9638:HOH:O	2.68	0.41
2:C:547:ILE:HA	2:C:548:PRO:HD3	1.96	0.41
3:N:589:ALA:N	9:N:2734:HOH:O	2.54	0.41
2:C:778:PHE:HE1	5:F:418:LEU:O	2.04	0.41
3:D:1097:LYS:HE2	9:D:9630:HOH:O	2.21	0.40
3:D:1093:TYR:O	3:D:1097:LYS:HG2	2.21	0.40
2:C:628:PHE:HA	9:C:2384:HOH:O	2.21	0.40
3:D:764:LEU:HG	3:D:765:SER:N	2.36	0.40
3:N:128:TYR:O	3:N:568:ARG:NH2	2.54	0.40
2:M:321:GLU:HB3	9:M:9404:HOH:O	2.20	0.40
3:N:824:ASN:ND2	9:N:9277:HOH:O	2.53	0.40
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.52	0.40
2:M:157:ARG:HB3	9:M:2325:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.81	0.40
1:K:5:LYS:NZ	9:K:1872:HOH:O	2.54	0.40
1:K:5:LYS:O	1:K:8:ALA:HB2	2.21	0.40
2:C:162:ILE:O	2:C:164:PRO:HD3	2.21	0.40
2:C:266:ARG:HD3	2:C:288:ARG:NE	2.32	0.40
2:C:287:GLY:O	2:C:288:ARG:C	2.59	0.40
2:C:482:GLU:HG2	2:C:483:VAL:N	2.36	0.40
2:C:471:TYR:HE1	2:C:491:GLU:HG3	1.86	0.40
3:D:998:GLU:HG2	9:D:3028:HOH:O	2.21	0.40
2:M:1086:ARG:HG3	2:M:1086:ARG:NH1	2.36	0.40
5:P:94:LEU:HD12	5:P:97:GLU:CB	2.50	0.40
1:A:132:LEU:HD23	1:A:136:GLY:O	2.22	0.40
3:D:1343:ALA:N	9:D:9670:HOH:O	2.54	0.40
3:N:221:ALA:HB3	3:N:367:ILE:CB	2.52	0.40
3:D:470:LEU:HD22	3:D:499:VAL:HG13	2.02	0.40
2:C:193:LEU:HD12	2:C:307:LEU:HD22	2.03	0.40
1:B:90:LEU:HD22	9:B:9609:HOH:O	2.21	0.40
3:D:1112:CYS:HB2	9:D:9694:HOH:O	2.21	0.40
9:C:9574:HOH:O	3:D:582:LEU:HD21	2.21	0.40
2:M:44:ILE:HD12	2:M:44:ILE:N	2.36	0.40
2:C:532:MET:HG3	2:C:533:ASP:N	2.36	0.40
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.55	0.40
2:C:927:GLY:HA3	9:C:2426:HOH:O	2.20	0.40
3:N:1308:GLU:HG2	9:N:2487:HOH:O	2.21	0.40
2:M:577:PRO:HG3	2:M:993:PHE:CD1	2.56	0.40
2:C:462:ASP:CG	2:C:468:ARG:HE	2.23	0.40
2:M:360:LEU:HD11	9:M:2160:HOH:O	2.19	0.40
3:D:493:ARG:HE	3:D:1389:LEU:HD21	1.86	0.40
3:N:1424:VAL:HG13	3:N:1425:THR:N	2.36	0.40
3:D:211:VAL:HG12	3:D:212:ARG:N	2.36	0.40
2:C:140:ILE:HD11	2:C:412:ALA:HB2	2.03	0.40
2:C:743:VAL:HG11	2:C:755:LEU:HD13	2.03	0.40
3:D:1198:TYR:OH	3:D:1394:VAL:HG21	2.21	0.40
2:M:786:LYS:NZ	9:M:2081:HOH:O	2.54	0.40
3:N:736:PHE:HA	9:N:9545:HOH:O	2.21	0.40
3:N:935:LYS:HG2	3:N:939:PHE:CE1	2.57	0.40
3:D:795:VAL:HA	3:D:861:GLN:O	2.22	0.40
5:F:373:LYS:HA	5:F:378:GLY:C	2.42	0.40
2:C:358:ARG:NH2	2:C:373:VAL:N	2.66	0.40
2:C:300:ASP:HB2	2:C:303:PHE:CD1	2.56	0.40
1:A:18:ARG:NH2	1:A:88:ARG:NH2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:ARG:CZ	9:K:2975:HOH:O	2.70	0.40
3:N:55:ASP:O	3:N:82:LYS:HA	2.22	0.40
1:L:13:VAL:HG12	1:L:14:ARG:N	2.36	0.40
5:F:78:SER:O	5:F:82:ARG:HG3	2.21	0.40
2:C:855:VAL:CG2	2:C:866:PRO:HG2	2.52	0.40
3:D:1278:ASP:N	3:D:1278:ASP:OD1	2.54	0.40
2:M:1107:ASN:HB3	9:M:9373:HOH:O	2.20	0.40
2:M:637:LEU:CD2	2:M:659:PRO:HG2	2.51	0.40
1:B:10:VAL:HG12	1:B:12:THR:HG23	2.02	0.40
2:M:609:ASN:HB3	9:M:9455:HOH:O	2.20	0.40
2:C:686:ASP:N	9:C:2345:HOH:O	2.53	0.40
2:M:44:ILE:HG23	9:M:9747:HOH:O	2.20	0.40
5:F:396:ARG:HB2	9:F:9739:HOH:O	2.21	0.40
3:N:671:LYS:HE3	5:P:421:PHE:O	2.22	0.40
2:C:917:LEU:HG	9:C:9726:HOH:O	2.21	0.40
5:F:256:ARG:HB3	9:F:9562:HOH:O	2.22	0.40
5:P:110:MET:HE2	9:P:2076:HOH:O	2.20	0.40
5:P:208:SER:HB2	5:P:211:ASP:OD1	2.20	0.40
3:D:70:GLY:HA3	9:D:2046:HOH:O	2.20	0.40
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.04	0.40
5:P:364:ARG:O	5:P:368:VAL:HG23	2.22	0.40
3:N:456:MET:CG	3:N:568:ARG:HD3	2.51	0.40
2:C:442:GLU:HG3	9:C:9844:HOH:O	2.21	0.40
3:N:983:LEU:HG	9:N:2329:HOH:O	2.21	0.40
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.36	0.40
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.51	0.40
2:M:724:ARG:HD2	2:M:738:ASP:O	2.21	0.40
2:M:737:LEU:O	2:M:738:ASP:C	2.59	0.40
2:C:1014:SER:HB2	5:F:331:ASP:OD1	2.21	0.40
3:N:64:LYS:HD3	5:P:376:ILE:O	2.21	0.40
3:D:806:PHE:HE1	3:D:813:LEU:HB3	1.84	0.40
1:A:146:ARG:HG3	9:A:9628:HOH:O	2.21	0.40
2:C:473:ARG:HH11	2:C:473:ARG:HG2	1.86	0.40
4:E:35:PHE:HE2	4:E:63:TRP:CD2	2.40	0.40
3:N:416:ALA:HA	3:N:442:ASN:ND2	2.36	0.40
5:F:234:LYS:CD	5:F:236:SER:HB2	2.49	0.40
1:L:104:GLU:HA	1:L:136:GLY:O	2.21	0.40
3:N:1345:GLU:HG2	3:N:1376:MET:SD	2.62	0.40
1:A:5:LYS:O	1:A:8:ALA:HB2	2.21	0.40
2:M:575:GLN:HE21	2:M:671:ASN:HD22	1.69	0.40
1:K:100:LEU:HD11	9:K:7148:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:719:PRO:HG3	9:M:9740:HOH:O	2.22	0.40
1:B:81:ASN:ND2	9:B:9670:HOH:O	2.54	0.40
3:D:1159:ARG:NH1	3:D:1159:ARG:HG3	2.35	0.40
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.22	0.40
3:N:96:ALA:CB	3:N:554:LEU:HG	2.51	0.40
5:P:392:VAL:CG1	5:P:396:ARG:HB2	2.51	0.40
2:C:636:ALA:C	2:C:637:LEU:HD23	2.41	0.40
2:M:49:ARG:HG2	9:M:2240:HOH:O	2.21	0.40
1:A:68:ILE:O	1:A:71:VAL:HB	2.21	0.40
2:M:44:ILE:HD12	2:M:44:ILE:H	1.86	0.40
3:N:115:LEU:HD12	9:N:9458:HOH:O	2.21	0.40
3:N:930:LEU:O	3:N:930:LEU:HD12	2.21	0.40
1:L:17:GLY:C	1:L:19:GLU:H	2.25	0.40
2:C:117:HIS:HB2	9:C:2237:HOH:O	2.21	0.40
2:C:280:LYS:HB3	9:C:2065:HOH:O	2.21	0.40
3:D:116:LEU:C	3:D:118:LEU:HD13	2.41	0.40
1:L:206:THR:HG22	1:L:209:GLU:H	1.86	0.40
2:M:516:ARG:HD2	3:N:1068:LEU:HD22	2.02	0.40
3:N:116:LEU:HB3	3:N:118:LEU:CD1	2.41	0.40
5:F:215:GLU:HA	5:F:215:GLU:OE1	2.21	0.40
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.57	0.40
2:C:551:GLU:HB2	9:C:9690:HOH:O	2.21	0.40
3:N:704:ARG:CG	3:N:705:ALA:N	2.84	0.40
2:M:413:LEU:HD22	9:M:2205:HOH:O	2.22	0.40
1:A:76:VAL:HA	1:A:79:ILE:HG12	2.03	0.40
1:K:196:THR:HG23	1:K:196:THR:O	2.20	0.40
1:K:57:TYR:CG	1:K:161:ARG:HD3	2.56	0.40
3:N:126:VAL:HG13	3:N:132:TYR:CB	2.49	0.40
3:N:601:ARG:NH2	3:N:613:ARG:NH2	2.69	0.40
1:B:170:VAL:N	9:B:9602:HOH:O	2.54	0.40
1:L:198:ARG:HG2	9:L:1453:HOH:O	2.21	0.40
5:F:93:LEU:HD11	5:F:187:LEU:HA	2.03	0.40
2:C:432:ARG:HG2	2:C:432:ARG:H	1.50	0.40
2:M:473:ARG:HH21	2:M:484:VAL:HG21	1.86	0.40
3:D:80:VAL:HA	9:D:9665:HOH:O	2.21	0.40
3:N:1087:ARG:HE	3:N:1238:MET:CB	2.34	0.40
3:D:789:LEU:CD1	3:D:934:LEU:HD22	2.51	0.40
4:O:25:LYS:HA	4:O:28:GLN:CD	2.41	0.40
4:O:10:PHE:O	4:O:13:VAL:HG22	2.22	0.40
3:D:995:LEU:HB3	9:D:2129:HOH:O	2.20	0.40
3:D:586:ARG:NE	9:D:2208:HOH:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:2038:HOH:O	3:N:680:GLN:HB2	2.22	0.40
5:P:253:ASP:HB3	5:P:259:ARG:NH2	2.36	0.40
2:C:427:VAL:HG22	9:C:2153:HOH:O	2.20	0.40
5:P:294:ALA:HA	9:P:4602:HOH:O	2.21	0.40
3:D:836:VAL:HA	3:D:839:LEU:HD12	2.03	0.40
3:N:239:GLY:HA2	9:N:9367:HOH:O	2.21	0.40
2:C:122:THR:HG22	2:C:123:GLU:N	2.37	0.40
3:D:683:ILE:HB	9:D:9721:HOH:O	2.22	0.40
3:D:702:LEU:N	3:D:702:LEU:HD12	2.36	0.40
3:N:1378:TYR:CE2	3:N:1394:VAL:HG22	2.56	0.40
2:M:837:ASP:O	2:M:849:VAL:HG23	2.21	0.40
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.56	0.40
2:M:906:PHE:CD1	3:N:1067:VAL:HG22	2.57	0.40
5:F:316:SER:HB3	5:F:319:THR:OG1	2.22	0.40
2:C:829:GLN:HB2	9:C:9705:HOH:O	2.20	0.40
3:N:49:ILE:HD13	9:N:9259:HOH:O	2.22	0.40
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.51	0.40
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.57	0.40
2:M:1005:MET:HG3	3:N:629:SER:CB	2.44	0.40
2:C:724:ARG:O	2:C:734:LEU:HD11	2.21	0.40
3:N:1121:PRO:HG3	9:N:9490:HOH:O	2.21	0.40
1:K:9:PRO:HD2	1:L:224:TYR:CG	2.56	0.40
1:K:85:LEU:HD12	1:K:124:ASN:CB	2.51	0.40
3:D:729:HIS:CE1	3:D:730:PRO:HG2	2.57	0.40
2:C:739:GLU:N	9:C:9982:HOH:O	2.55	0.40
3:D:1440:PHE:O	3:D:1443:THR:HG23	2.21	0.40
3:D:554:LEU:O	3:D:557:LEU:HB2	2.20	0.40
2:C:435:TYR:HD1	3:D:1071:PHE:CE2	2.40	0.40
2:M:958:THR:O	2:M:962:GLN:HG3	2.22	0.40
2:M:881:ASN:N	2:M:881:ASN:HD22	2.11	0.40
3:D:1489:GLN:NE2	3:D:1489:GLN:HA	2.35	0.40
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.56	0.40
2:C:420:ARG:HA	9:C:2134:HOH:O	2.20	0.40
5:P:350:LEU:HG	5:P:354:LEU:CD1	2.50	0.40
5:F:281:GLU:HB2	9:F:9741:HOH:O	2.21	0.40
3:D:1192:LEU:N	9:D:9658:HOH:O	2.54	0.40
3:N:190:GLU:HG3	3:N:210:ARG:NH1	2.35	0.40
2:M:722:ILE:HD12	2:M:823:VAL:HG21	2.03	0.40
2:C:216:GLU:O	2:C:219:GLN:HG3	2.21	0.40
2:M:631:SER:OG	2:M:635:THR:N	2.55	0.40
3:D:175:VAL:HG21	9:D:3255:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1478:SER:O	3:N:1480:PHE:N	2.54	0.40
3:N:1417:TRP:HA	9:N:9243:HOH:O	2.21	0.40
1:K:185:ARG:O	1:K:185:ARG:HD2	2.22	0.40
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	187 (82%)	33 (14%)	7 (3%)	5	12
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	7	16
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	4	8
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	8	22
2	C	1117/1119 (100%)	856 (77%)	194 (17%)	67 (6%)	2	3
2	M	1117/1119 (100%)	863 (77%)	187 (17%)	67 (6%)	2	3
3	D	1388/1524 (91%)	1047 (75%)	248 (18%)	93 (7%)	1	2
3	N	1388/1524 (91%)	1042 (75%)	251 (18%)	95 (7%)	1	2
4	E	93/99 (94%)	72 (77%)	11 (12%)	10 (11%)	0	0
4	O	93/99 (94%)	70 (75%)	13 (14%)	10 (11%)	0	0
5	F	341/423 (81%)	264 (77%)	53 (16%)	24 (7%)	1	2
5	P	341/423 (81%)	267 (78%)	53 (16%)	21 (6%)	2	2
All	All	6786/7590 (89%)	5222 (77%)	1150 (17%)	414 (6%)	2	3

All (414) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	188	GLN
1	B	118	ALA
2	C	10	ARG
2	C	59	LYS
2	C	111	ASP
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	251	ASP
2	C	253	ALA
2	C	261	ILE
2	C	265	ARG
2	C	267	TYR
2	C	290	LEU
2	C	316	GLY
2	C	363	SER
2	C	369	PRO
2	C	419	THR
2	C	462	ASP
2	C	518	LYS
2	C	627	ARG
2	C	684	PHE
2	C	735	ARG
2	C	738	ASP
2	C	740	GLU
2	C	762	LYS
2	C	864	GLY
2	C	905	ILE
3	D	55	ASP
3	D	83	SER
3	D	98	PRO
3	D	120	ALA
3	D	136	ASP
3	D	140	ALA
3	D	177	ALA
3	D	208	PRO
3	D	209	ARG
3	D	233	LYS
3	D	234	GLU
3	D	238	PRO
3	D	246	PRO

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Mol	Chain	Res	Type
3	D	370	ALA
3	D	373	PRO
3	D	385	VAL
3	D	417	PRO
3	D	487	ALA
3	D	807	ALA
3	D	832	ARG
3	D	1028	ALA
3	D	1125	PRO
3	D	1197	ARG
3	D	1208	ASP
3	D	1243	THR
3	D	1388	ARG
3	D	1389	LEU
3	D	1390	LEU
4	E	42	PRO
4	E	58	PRO
5	F	75	ILE
5	F	76	SER
5	F	77	THR
5	F	145	PRO
5	F	148	LYS
5	F	153	PRO
5	F	297	PRO
5	F	324	GLU
5	F	341	PRO
5	F	364	ARG
5	F	390	PHE
1	K	118	ALA
1	K	187	GLY
1	L	118	ALA
2	M	10	ARG
2	M	59	LYS
2	M	111	ASP
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	251	ASP
2	M	253	ALA
2	M	261	ILE
2	M	265	ARG

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Mol	Chain	Res	Type
2	M	267	TYR
2	M	290	LEU
2	M	316	GLY
2	M	363	SER
2	M	369	PRO
2	M	419	THR
2	M	462	ASP
2	M	518	LYS
2	M	627	ARG
2	M	684	PHE
2	M	735	ARG
2	M	738	ASP
2	M	740	GLU
2	M	762	LYS
2	M	864	GLY
2	M	905	ILE
3	N	40	GLU
3	N	55	ASP
3	N	120	ALA
3	N	136	ASP
3	N	140	ALA
3	N	177	ALA
3	N	208	PRO
3	N	209	ARG
3	N	233	LYS
3	N	234	GLU
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	417	PRO
3	N	487	ALA
3	N	807	ALA
3	N	832	ARG
3	N	1028	ALA
3	N	1066	THR
3	N	1125	PRO
3	N	1197	ARG
3	N	1208	ASP
3	N	1243	THR
3	N	1287	GLU

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Mol	Chain	Res	Type
3	N	1389	LEU
3	N	1390	LEU
4	O	42	PRO
4	O	58	PRO
5	P	75	ILE
5	P	76	SER
5	P	77	THR
5	P	145	PRO
5	P	148	LYS
5	P	153	PRO
5	P	232	ARG
5	P	297	PRO
5	P	324	GLU
5	P	341	PRO
5	P	364	ARG
5	P	390	PHE
1	A	11	PHE
1	A	187	GLY
1	A	191	ASP
2	C	7	GLY
2	C	11	GLU
2	C	129	ILE
2	C	144	PRO
2	C	262	ALA
2	C	288	ARG
2	C	292	ARG
2	C	465	GLY
2	C	548	PRO
2	C	575	GLN
2	C	598	GLU
2	C	626	ARG
2	C	727	PRO
2	C	1005	MET
2	C	1016	ILE
2	C	1106	ASP
3	D	37	LEU
3	D	40	GLU
3	D	43	GLY
3	D	88	TYR
3	D	119	SER
3	D	135	LEU
3	D	202	VAL

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Mol	Chain	Res	Type
3	D	424	GLY
3	D	440	VAL
3	D	601	ARG
3	D	782	SER
3	D	1066	THR
3	D	1067	VAL
3	D	1111	ASP
3	D	1127	GLU
3	D	1129	THR
3	D	1265	ALA
3	D	1287	GLU
3	D	1475	GLY
4	E	43	GLU
5	F	147	LEU
5	F	232	ARG
5	F	255	ALA
1	K	188	GLN
2	M	7	GLY
2	M	11	GLU
2	M	23	VAL
2	M	129	ILE
2	M	130	ASN
2	M	262	ALA
2	M	292	ARG
2	M	465	GLY
2	M	548	PRO
2	M	598	GLU
2	M	626	ARG
2	M	727	PRO
2	M	1005	MET
2	M	1016	ILE
2	M	1106	ASP
3	N	37	LEU
3	N	43	GLY
3	N	82	LYS
3	N	83	SER
3	N	88	TYR
3	N	98	PRO
3	N	119	SER
3	N	135	LEU
3	N	202	VAL
3	N	217	LYS

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Mol	Chain	Res	Type
3	N	424	GLY
3	N	440	VAL
3	N	601	ARG
3	N	782	SER
3	N	1067	VAL
3	N	1089	ALA
3	N	1111	ASP
3	N	1127	GLU
3	N	1137	ARG
3	N	1265	ALA
3	N	1385	GLY
3	N	1388	ARG
3	N	1475	GLY
4	O	43	GLU
5	P	95	THR
5	P	420	ASP
2	C	130	ASN
2	C	164	PRO
2	C	170	PRO
2	C	457	ALA
2	C	739	GLU
2	C	767	PRO
2	C	1079	PRO
3	D	110	SER
3	D	115	LEU
3	D	117	ASP
3	D	137	PRO
3	D	190	GLU
3	D	410	SER
3	D	416	ALA
3	D	504	ASP
3	D	521	PRO
3	D	594	PRO
3	D	705	ALA
3	D	922	LEU
3	D	1089	ALA
3	D	1385	GLY
3	D	1429	LEU
4	E	5	GLY
4	E	33	HIS
4	E	41	GLU
4	E	46	PRO

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Mol	Chain	Res	Type
5	F	95	THR
5	F	286	PRO
5	F	420	ASP
5	F	421	PHE
1	K	11	PHE
1	L	191	ASP
2	M	144	PRO
2	M	164	PRO
2	M	170	PRO
2	M	223	ASP
2	M	288	ARG
2	M	381	ALA
2	M	457	ALA
2	M	699	PHE
2	M	739	GLU
2	M	767	PRO
3	N	115	LEU
3	N	137	PRO
3	N	189	GLN
3	N	206	ARG
3	N	410	SER
3	N	416	ALA
3	N	594	PRO
3	N	705	ALA
3	N	869	MET
3	N	922	LEU
3	N	1429	LEU
4	O	5	GLY
4	O	33	HIS
4	O	41	GLU
4	O	46	PRO
5	P	147	LEU
5	P	255	ALA
5	P	285	GLU
5	P	286	PRO
5	P	329	TYR
1	A	59	GLU
1	B	11	PHE
1	B	59	GLU
1	B	191	ASP
2	C	23	VAL
2	C	277	ALA

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Mol	Chain	Res	Type
2	C	381	ALA
2	C	415	PRO
2	C	699	PHE
3	D	31	THR
3	D	82	LYS
3	D	189	GLN
3	D	206	ARG
3	D	381	ALA
3	D	560	GLN
3	D	808	THR
3	D	869	MET
3	D	919	PHE
3	D	1051	GLU
3	D	1155	VAL
3	D	1248	GLY
3	D	1288	GLU
4	E	82	GLU
5	F	155	THR
5	F	285	GLU
5	F	329	TYR
1	K	59	GLU
1	K	191	ASP
1	L	11	PHE
1	L	59	GLU
2	M	277	ALA
2	M	415	PRO
2	M	1079	PRO
3	N	110	SER
3	N	133	ILE
3	N	149	LYS
3	N	190	GLU
3	N	504	ASP
3	N	521	PRO
3	N	560	GLN
3	N	801	GLY
3	N	806	PHE
3	N	808	THR
3	N	936	TYR
3	N	1051	GLU
3	N	1155	VAL
3	N	1248	GLY
5	P	416	ARG

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Mol	Chain	Res	Type
1	A	106	PRO
1	B	106	PRO
2	C	113	VAL
2	C	180	GLY
2	C	377	PRO
3	D	149	LYS
3	D	522	PRO
3	D	801	GLY
3	D	822	ALA
4	E	32	ARG
4	E	57	ASP
5	F	97	GLU
5	F	416	ARG
1	K	93	SER
1	K	106	PRO
2	M	180	GLY
2	M	434	HIS
2	M	1004	LYS
3	N	31	THR
3	N	522	PRO
3	N	822	ALA
3	N	919	PHE
3	N	945	SER
3	N	1019	PRO
4	O	32	ARG
4	O	57	ASP
4	O	82	GLU
2	C	202	TYR
2	C	1020	PRO
3	D	133	ILE
3	D	138	LYS
3	D	936	TYR
3	D	1213	ARG
1	K	172	SER
1	L	106	PRO
2	M	113	VAL
2	M	377	PRO
2	M	575	GLN
3	N	117	ASP
3	N	381	ALA
3	N	406	ASP
3	N	1205	TYR

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Mol	Chain	Res	Type
3	N	1213	ARG
5	P	167	PRO
2	C	779	GLY
3	D	245	LEU
3	D	509	PRO
3	D	1019	PRO
5	F	167	PRO
2	M	777	ILE
2	M	779	GLY
1	B	48	ILE
2	C	42	VAL
3	D	141	ILE
2	M	1020	PRO
3	N	245	LEU
2	C	811	PRO
2	C	876	VAL
3	D	175	VAL
2	M	42	VAL
2	M	876	VAL
3	N	78	VAL
3	N	108	VAL
3	N	141	ILE
3	N	173	PRO
2	C	777	ILE
3	D	78	VAL
3	D	425	GLY
3	D	670	VAL
3	N	425	GLY
3	N	526	PRO
2	C	1060	ILE
3	D	52	PRO
3	D	530	VAL
3	N	175	VAL
2	M	166	PRO
2	C	166	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	181 (90%)	21 (10%)	9	20
1	B	202/273 (74%)	186 (92%)	16 (8%)	15	34
1	K	202/273 (74%)	187 (93%)	15 (7%)	17	39
1	L	202/273 (74%)	190 (94%)	12 (6%)	24	51
2	C	941/941 (100%)	827 (88%)	114 (12%)	6	14
2	M	941/941 (100%)	838 (89%)	103 (11%)	8	18
3	D	1123/1279 (88%)	992 (88%)	131 (12%)	7	15
3	N	1123/1279 (88%)	987 (88%)	136 (12%)	6	14
4	E	83/87 (95%)	73 (88%)	10 (12%)	6	14
4	O	83/87 (95%)	73 (88%)	10 (12%)	6	14
5	F	295/370 (80%)	263 (89%)	32 (11%)	8	18
5	P	295/370 (80%)	273 (92%)	22 (8%)	17	38
All	All	5692/6446 (88%)	5070 (89%)	622 (11%)	8	18

All (622) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	5	LYS
1	A	9	PRO
1	A	15	THR
1	A	26	GLU
1	A	62	LEU
1	A	92	PRO
1	A	95	GLN
1	A	96	THR
1	A	124	ASN
1	A	145	ASP
1	A	146	ARG
1	A	156	HIS
1	A	160	ASP
1	A	170	VAL
1	A	185	ARG
1	A	196	THR
1	A	197	LEU
1	A	206	THR
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	227	ASN
1	B	7	LYS
1	B	9	PRO
1	B	26	GLU
1	B	62	LEU
1	B	95	GLN
1	B	96	THR
1	B	119	ASP
1	B	124	ASN
1	B	134	GLU
1	B	138	LEU
1	B	140	MET
1	B	145	ASP
1	B	159	LYS
1	B	160	ASP
1	B	189	ARG
1	B	206	THR
2	C	6	PHE
2	C	8	ARG
2	C	26	TYR
2	C	30	LEU
2	C	41	ASN
2	C	48	PHE
2	C	52	PHE
2	C	81	ASP
2	C	87	ASP
2	C	95	TYR
2	C	107	LEU
2	C	113	VAL
2	C	114	PHE
2	C	115	LEU
2	C	118	ILE
2	C	134	ARG
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	168	ARG
2	C	178	PRO
2	C	184	MET
2	C	186	VAL
2	C	190	LYS

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Mol	Chain	Res	Type
2	C	198	ARG
2	C	203	ASP
2	C	207	LEU
2	C	216	GLU
2	C	217	LEU
2	C	218	VAL
2	C	224	GLU
2	C	243	ARG
2	C	246	ASP
2	C	247	PRO
2	C	256	TYR
2	C	261	ILE
2	C	266	ARG
2	C	268	ASP
2	C	281	LEU
2	C	288	ARG
2	C	289	THR
2	C	290	LEU
2	C	309	TYR
2	C	321	GLU
2	C	333	ILE
2	C	344	PHE
2	C	359	MET
2	C	367	LEU
2	C	388	ARG
2	C	389	SER
2	C	393	GLN
2	C	402	SER
2	C	418	LEU
2	C	420	ARG
2	C	425	PHE
2	C	432	ARG
2	C	455	LEU
2	C	460	ARG
2	C	469	THR
2	C	471	TYR
2	C	500	ASN
2	C	507	ARG
2	C	527	GLU
2	C	533	ASP
2	C	559	LEU
2	C	564	MET

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Mol	Chain	Res	Type
2	C	579	VAL
2	C	584	GLU
2	C	620	LEU
2	C	627	ARG
2	C	637	LEU
2	C	640	ARG
2	C	645	VAL
2	C	650	ARG
2	C	657	ASP
2	C	689	VAL
2	C	693	GLU
2	C	699	PHE
2	C	701	THR
2	C	719	PRO
2	C	727	PRO
2	C	739	GLU
2	C	744	ARG
2	C	755	LEU
2	C	773	LEU
2	C	785	VAL
2	C	807	ARG
2	C	815	LEU
2	C	824	ARG
2	C	841	ASN
2	C	862	PRO
2	C	865	THR
2	C	881	ASN
2	C	886	LEU
2	C	887	GLU
2	C	900	ARG
2	C	917	LEU
2	C	934	PHE
2	C	945	ARG
2	C	950	LEU
2	C	952	LEU
2	C	959	PRO
2	C	962	GLN
2	C	982	PRO
2	C	988	VAL
2	C	999	HIS
2	C	1003	ASP
2	C	1016	ILE

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Mol	Chain	Res	Type
2	C	1017	THR
2	C	1019	GLN
2	C	1020	PRO
2	C	1052	MET
2	C	1115	LEU
3	D	3	LYS
3	D	6	ARG
3	D	12	LEU
3	D	25	GLU
3	D	27	GLU
3	D	42	ASP
3	D	56	TYR
3	D	66	GLN
3	D	76	CYS
3	D	87	ARG
3	D	98	PRO
3	D	103	TRP
3	D	121	THR
3	D	127	LEU
3	D	135	LEU
3	D	136	ASP
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	163	TYR
3	D	168	THR
3	D	169	TYR
3	D	171	LEU
3	D	185	VAL
3	D	199	LEU
3	D	208	PRO
3	D	389	GLU
3	D	393	ILE
3	D	403	PHE
3	D	423	ASP
3	D	426	LYS
3	D	445	ARG
3	D	447	VAL
3	D	456	MET
3	D	465	LEU
3	D	476	GLU
3	D	486	ARG

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Mol	Chain	Res	Type
3	D	488	ARG
3	D	521	PRO
3	D	523	ASP
3	D	528	VAL
3	D	554	LEU
3	D	569	ASN
3	D	594	PRO
3	D	602	SER
3	D	605	ASP
3	D	624	ASP
3	D	626	SER
3	D	629	SER
3	D	635	PRO
3	D	651	GLU
3	D	662	GLU
3	D	676	MET
3	D	679	ARG
3	D	685	ASP
3	D	710	ARG
3	D	725	SER
3	D	727	GLN
3	D	754	PHE
3	D	770	LEU
3	D	781	PRO
3	D	782	SER
3	D	792	ILE
3	D	794	GLN
3	D	796	ARG
3	D	828	LYS
3	D	829	VAL
3	D	834	THR
3	D	863	VAL
3	D	865	THR
3	D	873	LEU
3	D	899	LEU
3	D	904	VAL
3	D	935	LYS
3	D	961	LYS
3	D	986	ARG
3	D	988	ARG
3	D	1029	ARG
3	D	1044	LEU

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Mol	Chain	Res	Type
3	D	1046	GLN
3	D	1058	ARG
3	D	1062	ARG
3	D	1096	ARG
3	D	1097	LYS
3	D	1109	GLU
3	D	1112	CYS
3	D	1127	GLU
3	D	1134	LEU
3	D	1135	ARG
3	D	1152	GLU
3	D	1159	ARG
3	D	1166	LEU
3	D	1182	GLU
3	D	1183	ILE
3	D	1194	CYS
3	D	1196	THR
3	D	1207	TYR
3	D	1209	LEU
3	D	1211	MET
3	D	1213	ARG
3	D	1231	GLU
3	D	1238	MET
3	D	1243	THR
3	D	1252	ILE
3	D	1253	THR
3	D	1257	PRO
3	D	1267	ARG
3	D	1278	ASP
3	D	1285	GLU
3	D	1299	PHE
3	D	1304	LYS
3	D	1306	PRO
3	D	1314	LYS
3	D	1315	ASP
3	D	1317	ASP
3	D	1326	THR
3	D	1337	GLU
3	D	1344	VAL
3	D	1346	ARG
3	D	1375	MET
3	D	1388	ARG

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Mol	Chain	Res	Type
3	D	1389	LEU
3	D	1390	LEU
3	D	1396	GLU
3	D	1406	ARG
3	D	1412	LYS
3	D	1427	SER
3	D	1432	LYS
3	D	1434	TRP
3	D	1442	ASN
3	D	1487	VAL
4	E	42	PRO
4	E	46	PRO
4	E	47	LYS
4	E	51	LEU
4	E	57	ASP
4	E	58	PRO
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	79	LEU
5	F	84	TYR
5	F	87	GLU
5	F	94	LEU
5	F	120	THR
5	F	124	PRO
5	F	125	ASP
5	F	142	ARG
5	F	149	GLU
5	F	156	VAL
5	F	174	LEU
5	F	203	THR
5	F	234	LYS
5	F	280	GLN
5	F	282	LEU
5	F	285	GLU
5	F	295	MET
5	F	297	PRO
5	F	307	THR
5	F	312	GLN
5	F	341	PRO
5	F	347	GLN
5	F	352	GLU

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Mol	Chain	Res	Type
5	F	361	LEU
5	F	362	SER
5	F	364	ARG
5	F	370	LYS
5	F	375	LEU
5	F	392	VAL
5	F	396	ARG
5	F	398	ARG
5	F	405	LEU
5	F	409	LYS
1	K	12	THR
1	K	15	THR
1	K	26	GLU
1	K	62	LEU
1	K	95	GLN
1	K	96	THR
1	K	124	ASN
1	K	143	ARG
1	K	146	ARG
1	K	167	VAL
1	K	186	LEU
1	K	201	THR
1	K	216	GLU
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	2	LEU
1	L	3	ASP
1	L	5	LYS
1	L	26	GLU
1	L	62	LEU
1	L	95	GLN
1	L	96	THR
1	L	124	ASN
1	L	145	ASP
1	L	189	ARG
1	L	196	THR
2	M	26	TYR
2	M	28	ARG
2	M	30	LEU
2	M	31	GLN
2	M	34	VAL

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Mol	Chain	Res	Type
2	M	39	ARG
2	M	41	ASN
2	M	52	PHE
2	M	68	PHE
2	M	107	LEU
2	M	115	LEU
2	M	129	ILE
2	M	144	PRO
2	M	147	TYR
2	M	152	PRO
2	M	158	TYR
2	M	167	LYS
2	M	168	ARG
2	M	170	PRO
2	M	178	PRO
2	M	185	LYS
2	M	186	VAL
2	M	189	ARG
2	M	194	VAL
2	M	198	ARG
2	M	203	ASP
2	M	207	LEU
2	M	209	ARG
2	M	216	GLU
2	M	221	LEU
2	M	230	ARG
2	M	243	ARG
2	M	254	VAL
2	M	256	TYR
2	M	257	VAL
2	M	288	ARG
2	M	290	LEU
2	M	309	TYR
2	M	328	LEU
2	M	333	ILE
2	M	343	GLN
2	M	359	MET
2	M	384	GLU
2	M	393	GLN
2	M	397	GLU
2	M	407	LYS
2	M	418	LEU

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Mol	Chain	Res	Type
2	M	420	ARG
2	M	426	ASP
2	M	432	ARG
2	M	455	LEU
2	M	481	ASP
2	M	503	LEU
2	M	523	ILE
2	M	533	ASP
2	M	542	VAL
2	M	548	PRO
2	M	564	MET
2	M	607	ASP
2	M	609	ASN
2	M	620	LEU
2	M	629	TYR
2	M	633	GLN
2	M	650	ARG
2	M	663	ASN
2	M	678	PRO
2	M	679	PHE
2	M	680	ASP
2	M	686	ASP
2	M	701	THR
2	M	716	LYS
2	M	727	PRO
2	M	728	HIS
2	M	729	LEU
2	M	737	LEU
2	M	750	LYS
2	M	765	SER
2	M	774	LEU
2	M	785	VAL
2	M	799	ILE
2	M	839	LEU
2	M	841	ASN
2	M	848	VAL
2	M	865	THR
2	M	871	LEU
2	M	876	VAL
2	M	881	ASN
2	M	886	LEU
2	M	928	LYS

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Mol	Chain	Res	Type
2	M	937	ASP
2	M	948	GLU
2	M	950	LEU
2	M	958	THR
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	1015	LEU
2	M	1026	GLN
2	M	1057	SER
2	M	1079	PRO
2	M	1098	ASP
2	M	1110	ASP
2	M	1119	ARG
3	N	12	LEU
3	N	19	ARG
3	N	23	TYR
3	N	25	GLU
3	N	34	TYR
3	N	47	GLU
3	N	65	ARG
3	N	71	LYS
3	N	76	CYS
3	N	98	PRO
3	N	109	PRO
3	N	115	LEU
3	N	122	GLU
3	N	126	VAL
3	N	128	TYR
3	N	131	LYS
3	N	135	LEU
3	N	138	LYS
3	N	142	LEU
3	N	143	ASN
3	N	145	VAL
3	N	149	LYS
3	N	154	THR
3	N	155	ASP
3	N	168	THR
3	N	185	VAL
3	N	190	GLU
3	N	197	SER

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Mol	Chain	Res	Type
3	N	199	LEU
3	N	205	TYR
3	N	208	PRO
3	N	394	LEU
3	N	403	PHE
3	N	406	ASP
3	N	432	TYR
3	N	442	ASN
3	N	445	ARG
3	N	452	ILE
3	N	456	MET
3	N	474	GLU
3	N	502	PHE
3	N	503	LEU
3	N	510	GLU
3	N	513	ILE
3	N	521	PRO
3	N	549	ASN
3	N	554	LEU
3	N	581	LEU
3	N	594	PRO
3	N	601	ARG
3	N	602	SER
3	N	604	THR
3	N	605	ASP
3	N	611	GLN
3	N	624	ASP
3	N	644	LEU
3	N	660	LYS
3	N	676	MET
3	N	679	ARG
3	N	681	ARG
3	N	682	ASP
3	N	703	ASN
3	N	707	THR
3	N	709	HIS
3	N	711	LEU
3	N	722	GLU
3	N	724	GLN
3	N	737	ASN
3	N	739	ASP
3	N	754	PHE

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Mol	Chain	Res	Type
3	N	794	GLN
3	N	800	LYS
3	N	828	LYS
3	N	845	ASN
3	N	847	ASP
3	N	859	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	879	ARG
3	N	880	ILE
3	N	897	TRP
3	N	899	LEU
3	N	902	LEU
3	N	907	GLU
3	N	919	PHE
3	N	942	SER
3	N	951	ILE
3	N	970	LYS
3	N	1005	GLN
3	N	1029	ARG
3	N	1045	MET
3	N	1058	ARG
3	N	1062	ARG
3	N	1066	THR
3	N	1068	LEU
3	N	1083	ASP
3	N	1087	ARG
3	N	1096	ARG
3	N	1109	GLU
3	N	1112	CYS
3	N	1124	GLN
3	N	1127	GLU
3	N	1134	LEU
3	N	1137	ARG
3	N	1164	ARG
3	N	1166	LEU
3	N	1169	ASP
3	N	1183	ILE
3	N	1197	ARG
3	N	1207	TYR
3	N	1211	MET

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Mol	Chain	Res	Type
3	N	1231	GLU
3	N	1243	THR
3	N	1252	ILE
3	N	1253	THR
3	N	1267	ARG
3	N	1274	ILE
3	N	1278	ASP
3	N	1285	GLU
3	N	1287	GLU
3	N	1297	GLU
3	N	1304	LYS
3	N	1308	GLU
3	N	1311	LEU
3	N	1314	LYS
3	N	1318	TYR
3	N	1342	GLU
3	N	1350	GLU
3	N	1376	MET
3	N	1389	LEU
3	N	1396	GLU
3	N	1415	VAL
3	N	1442	ASN
3	N	1468	LEU
3	N	1497	GLU
4	O	3	GLU
4	O	32	ARG
4	O	40	LEU
4	O	42	PRO
4	O	46	PRO
4	O	51	LEU
4	O	58	PRO
4	O	59	ASN
4	O	61	GLU
4	O	85	LEU
5	P	84	TYR
5	P	86	HIS
5	P	91	VAL
5	P	120	THR
5	P	122	LEU
5	P	142	ARG
5	P	148	LYS
5	P	149	GLU

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Mol	Chain	Res	Type
5	P	174	LEU
5	P	194	LEU
5	P	208	SER
5	P	280	GLN
5	P	281	GLU
5	P	295	MET
5	P	302	LYS
5	P	318	GLU
5	P	341	PRO
5	P	353	GLU
5	P	401	GLU
5	P	406	ARG
5	P	409	LYS
5	P	411	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	124	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	212	ASN
1	A	213	GLN
1	A	227	ASN
1	A	229	GLN
1	B	63	HIS
1	B	95	GLN
1	B	124	ASN
1	B	163	ASN
1	B	212	ASN
1	B	221	HIS
1	B	227	ASN
2	C	31	GLN
2	C	41	ASN
2	C	45	GLN
2	C	91	GLN
2	C	204	GLN
2	C	343	GLN
2	C	431	HIS
2	C	434	HIS

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Mol	Chain	Res	Type
2	C	498	GLN
2	C	538	GLN
2	C	552	HIS
2	C	609	ASN
2	C	632	ASN
2	C	671	ASN
2	C	704	HIS
2	C	829	GLN
2	C	834	GLN
2	C	841	ASN
2	C	843	HIS
2	C	881	ASN
2	C	889	HIS
2	C	969	GLN
2	C	991	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1100	GLN
3	D	166	GLN
3	D	507	ASN
3	D	549	ASN
3	D	575	GLN
3	D	616	GLN
3	D	669	ASN
3	D	696	HIS
3	D	717	GLN
3	D	744	GLN
3	D	756	GLN
3	D	768	ASN
3	D	816	HIS
3	D	824	ASN
3	D	845	ASN
3	D	962	GLN
3	D	976	GLN
3	D	991	GLN
3	D	994	GLN
3	D	1005	GLN
3	D	1124	GLN
3	D	1202	GLN
3	D	1465	ASN
3	D	1489	GLN
4	E	33	HIS

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Mol	Chain	Res	Type
4	E	86	GLN
5	F	90	GLN
5	F	191	ASN
5	F	217	ASN
5	F	218	GLN
5	F	245	GLN
5	F	269	ASN
5	F	337	HIS
5	F	402	ASN
1	K	81	ASN
1	K	95	GLN
1	K	124	ASN
1	K	163	ASN
1	K	180	GLN
1	K	212	ASN
1	K	227	ASN
1	L	81	ASN
1	L	95	GLN
1	L	124	ASN
1	L	163	ASN
1	L	180	GLN
1	L	221	HIS
1	L	229	GLN
2	M	31	GLN
2	M	41	ASN
2	M	80	GLN
2	M	99	GLN
2	M	187	ASN
2	M	204	GLN
2	M	330	ASN
2	M	343	GLN
2	M	390	GLN
2	M	431	HIS
2	M	434	HIS
2	M	538	GLN
2	M	545	ASN
2	M	552	HIS
2	M	565	GLN
2	M	567	GLN
2	M	575	GLN
2	M	663	ASN
2	M	829	GLN

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Mol	Chain	Res	Type
2	M	841	ASN
2	M	881	ASN
2	M	969	GLN
2	M	1018	GLN
2	M	1026	GLN
2	M	1050	GLN
2	M	1093	GLN
2	M	1107	ASN
3	N	101	HIS
3	N	151	GLN
3	N	166	GLN
3	N	442	ASN
3	N	462	GLN
3	N	529	GLN
3	N	552	ASN
3	N	569	ASN
3	N	575	GLN
3	N	636	GLN
3	N	703	ASN
3	N	709	HIS
3	N	724	GLN
3	N	727	GLN
3	N	737	ASN
3	N	744	GLN
3	N	756	GLN
3	N	767	HIS
3	N	768	ASN
3	N	794	GLN
3	N	901	GLN
3	N	962	GLN
3	N	991	GLN
3	N	994	GLN
3	N	1005	GLN
3	N	1010	ASN
3	N	1014	ASN
3	N	1184	GLN
3	N	1323	GLN
3	N	1442	ASN
3	N	1465	ASN
4	O	28	GLN
4	O	29	GLN
4	O	33	HIS

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Mol	Chain	Res	Type
4	O	37	ASN
5	P	83	GLN
5	P	90	GLN
5	P	161	GLN
5	P	191	ASN
5	P	254	GLN
5	P	277	GLN
5	P	280	GLN
5	P	312	GLN
5	P	337	HIS
5	P	399	GLN
5	P	411	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 368 ligands modelled in this entry, 366 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	G4P	N	9100	6	29,38,38	1.49	4 (13%)	42,61,61	2.32	11 (26%)
8	G4P	N	9101	6	29,38,38	1.66	6 (20%)	42,61,61	2.44	11 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	G4P	N	9100	6	-	0/23/43/43	0/3/3/3
8	G4P	N	9101	6	-	0/23/43/43	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9101	G4P	C8-N7	-2.53	1.29	1.34
8	N	9100	G4P	C8-N7	-2.50	1.29	1.34
8	N	9101	G4P	C2-N2	2.14	1.38	1.34
8	N	9101	G4P	PD-O3D	2.59	1.64	1.54
8	N	9101	G4P	C2-N1	2.70	1.40	1.35
8	N	9100	G4P	PD-O3D	2.94	1.65	1.54
8	N	9100	G4P	O4'-C1'	3.40	1.45	1.41
8	N	9100	G4P	C6-N1	4.06	1.40	1.33
8	N	9101	G4P	O4'-C1'	4.15	1.46	1.41
8	N	9101	G4P	C6-N1	5.37	1.43	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9100	G4P	C5-C6-N1	-8.54	111.91	123.59
8	N	9101	G4P	C5-C6-N1	-8.45	112.03	123.59
8	N	9101	G4P	C2'-C1'-N9	-5.39	106.05	114.29
8	N	9101	G4P	PC-O3C-PD	-5.37	114.65	132.67
8	N	9100	G4P	PA-O3A-PB	-4.45	117.73	132.67
8	N	9101	G4P	N3-C2-N1	-2.97	122.92	127.44
8	N	9100	G4P	N3-C2-N1	-2.78	123.22	127.44
8	N	9101	G4P	PA-O3A-PB	-2.49	124.33	132.67
8	N	9100	G4P	O3B-PB-O3A	-2.37	94.35	105.09
8	N	9100	G4P	O3'-PC-O1C	-2.25	100.61	109.46
8	N	9101	G4P	O2'-C2'-C3'	2.06	117.11	111.16
8	N	9101	G4P	C2'-C3'-C4'	2.10	107.24	103.29
8	N	9100	G4P	O3'-C3'-C4'	2.17	118.52	109.99
8	N	9100	G4P	O3'-C3'-C2'	2.33	120.57	111.51
8	N	9101	G4P	C4-C5-N7	2.34	111.63	109.48
8	N	9101	G4P	O4'-C1'-N9	2.42	113.16	108.10
8	N	9100	G4P	O3B-PB-O1B	2.68	119.20	110.58
8	N	9100	G4P	O5'-PA-O1A	2.68	120.03	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	N	9100	G4P	C2'-C3'-C4'	2.85	108.65	103.29
8	N	9101	G4P	O3'-C3'-C4'	3.94	125.47	109.99
8	N	9101	G4P	C6-N1-C2	6.09	124.39	115.94
8	N	9100	G4P	C6-N1-C2	6.47	124.92	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9100	G4P	4	0
8	N	9101	G4P	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.71	2 (0%) 85 86	39, 65, 90, 121	0
1	B	229/315 (72%)	-0.67	3 (1%) 79 79	58, 82, 103, 129	0
1	K	229/315 (72%)	-0.69	1 (0%) 93 94	42, 65, 87, 117	0
1	L	229/315 (72%)	-0.68	2 (0%) 85 86	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-0.77	1 (0%) 95 97	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-0.73	7 (0%) 90 91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-0.67	17 (1%) 81 81	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-0.69	18 (1%) 79 79	35, 71, 108, 145	0
4	E	95/99 (95%)	-0.87	0 100 100	49, 79, 103, 109	0
4	O	95/99 (95%)	-0.74	0 100 100	42, 81, 111, 119	0
5	F	345/423 (81%)	-0.58	7 (2%) 68 69	53, 84, 111, 126	0
5	P	345/423 (81%)	-0.63	2 (0%) 90 91	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-0.70	60 (0%) 85 86	30, 74, 108, 152	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1246	VAL	7.4
3	D	1245	GLY	7.3
3	D	1246	VAL	6.6
3	N	1247	ALA	6.3
1	K	1	MET	5.5
3	D	1243	THR	5.4
3	N	1245	GLY	5.2
3	N	407	VAL	4.9
3	D	1247	ALA	4.6
3	N	1244	GLY	4.5
3	D	1242	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.3
2	M	39	ARG	4.2
3	N	1242	HIS	4.2
3	N	1243	THR	4.2
1	B	2	LEU	4.0
5	F	389	PHE	3.9
1	L	97	VAL	3.7
2	M	269	LEU	3.5
2	M	268	ASP	3.5
3	D	1398	TRP	3.5
2	M	40	GLU	3.4
1	B	1	MET	3.4
2	C	39	ARG	3.3
3	D	1244	GLY	3.2
3	N	1408	ILE	3.1
1	A	2	LEU	3.0
3	D	1407	LEU	2.9
5	F	391	GLY	2.9
3	D	594	PRO	2.9
3	D	816	HIS	2.8
3	D	410	SER	2.7
5	P	365	GLU	2.7
5	F	394	ARG	2.6
3	D	1408	ILE	2.6
3	N	1241	PHE	2.6
3	D	1241	PHE	2.6
3	N	403	PHE	2.5
3	N	401	TYR	2.5
2	M	270	GLY	2.5
3	N	900	ILE	2.5
5	F	388	ALA	2.4
3	D	1240	THR	2.4
5	P	408	LEU	2.4
5	F	397	ILE	2.4
3	N	405	ASP	2.4
2	M	186	VAL	2.3
3	D	403	PHE	2.3
3	N	594	PRO	2.3
5	F	384	GLU	2.2
5	F	151	LEU	2.2
3	D	72	VAL	2.2
1	B	119	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	94	LEU	2.2
3	N	61	GLY	2.2
3	N	71	LYS	2.1
2	M	267	TYR	2.1
3	N	899	LEU	2.1
3	N	1305	LEU	2.0
3	D	68	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	A	9209	1/1	1.00	0.20	2.92	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.10	0.03	20,20,20,20	0
6	MG	F	9229	1/1	0.99	0.11	-0.14	20,20,20,20	0
6	MG	C	9438	1/1	0.99	0.11	-0.56	20,20,20,20	0
8	G4P	N	9101	36/36	0.99	0.11	-0.60	35,45,50,50	0
6	MG	D	9234	1/1	1.00	0.09	-0.61	20,20,20,20	0
8	G4P	N	9100	36/36	0.98	0.11	-0.66	35,45,54,55	0
7	ZN	N	9105	1/1	0.98	0.10	-0.72	80,80,80,80	0
7	ZN	D	9103	1/1	0.98	0.09	-0.88	87,87,87,87	0
6	MG	C	9346	1/1	1.00	0.10	-1.22	20,20,20,20	0
6	MG	C	9396	1/1	0.99	0.07	-1.39	20,20,20,20	0
6	MG	C	9282	1/1	0.99	0.05	-1.52	20,20,20,20	0
6	MG	D	9220	1/1	0.98	0.07	-1.54	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.11	-1.56	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9294	1/1	0.98	0.07	-1.56	20,20,20,20	0
6	MG	B	9235	1/1	0.98	0.06	-1.62	20,20,20,20	0
7	ZN	D	9102	1/1	0.96	0.06	-1.63	115,115,115,115	0
6	MG	C	9238	1/1	0.98	0.07	-1.67	20,20,20,20	0
6	MG	F	9374	1/1	0.99	0.05	-1.67	20,20,20,20	0
7	ZN	N	9104	1/1	0.98	0.05	-1.68	116,116,116,116	0
6	MG	F	9302	1/1	0.99	0.06	-1.70	20,20,20,20	0
6	MG	D	9225	1/1	0.99	0.06	-1.73	20,20,20,20	0
6	MG	F	9303	1/1	0.99	0.06	-1.77	20,20,20,20	0
6	MG	D	9353	1/1	0.99	0.05	-1.77	20,20,20,20	0
6	MG	D	9283	1/1	0.99	0.10	-1.78	20,20,20,20	0
6	MG	E	9432	1/1	0.99	0.06	-1.86	20,20,20,20	0
6	MG	F	9251	1/1	0.99	0.05	-1.92	20,20,20,20	0
6	MG	D	9218	1/1	0.99	0.07	-1.94	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.05	-1.99	20,20,20,20	0
6	MG	D	9236	1/1	0.99	0.08	-2.11	20,20,20,20	0
6	MG	B	9230	1/1	1.00	0.07	-2.14	20,20,20,20	0
6	MG	D	9523	1/1	0.99	0.09	-2.14	20,20,20,20	0
6	MG	F	9244	1/1	0.99	0.05	-2.40	20,20,20,20	0
6	MG	B	9427	1/1	0.99	0.04	-2.45	20,20,20,20	0
6	MG	D	9557	1/1	0.99	0.06	-2.47	20,20,20,20	0
6	MG	C	9507	1/1	0.99	0.03	-2.52	20,20,20,20	0
6	MG	D	9262	1/1	0.99	0.05	-2.55	20,20,20,20	0
6	MG	D	9247	1/1	0.99	0.07	-2.57	20,20,20,20	0
6	MG	D	9211	1/1	0.99	0.06	-2.72	20,20,20,20	0
6	MG	D	9253	1/1	0.99	0.08	-2.83	20,20,20,20	0
6	MG	C	9525	1/1	0.97	0.05	-2.86	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.05	-2.89	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.05	-2.90	20,20,20,20	0
6	MG	D	9480	1/1	0.98	0.07	-2.93	20,20,20,20	0
6	MG	C	9264	1/1	0.99	0.07	-3.06	20,20,20,20	0
6	MG	C	9210	1/1	0.98	0.05	-3.12	20,20,20,20	0
6	MG	C	9408	1/1	0.99	0.05	-3.20	20,20,20,20	0
6	MG	C	9221	1/1	0.99	0.07	-3.26	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.07	-3.36	20,20,20,20	0
6	MG	D	9386	1/1	0.98	0.04	-3.39	20,20,20,20	0
6	MG	A	9473	1/1	0.99	0.05	-3.42	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.04	-3.45	20,20,20,20	0
6	MG	B	9260	1/1	0.99	0.05	-3.63	20,20,20,20	0
6	MG	D	9419	1/1	0.99	0.05	-3.67	20,20,20,20	0
6	MG	D	9233	1/1	0.99	0.06	-3.78	20,20,20,20	0
6	MG	D	9277	1/1	0.99	0.09	-3.83	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9300	1/1	0.99	0.03	-3.87	20,20,20,20	0
6	MG	C	9287	1/1	0.99	0.04	-3.91	20,20,20,20	0
6	MG	D	9307	1/1	1.00	0.06	-4.11	20,20,20,20	0
6	MG	C	9263	1/1	0.99	0.08	-4.20	20,20,20,20	0
6	MG	A	9227	1/1	0.99	0.05	-4.21	20,20,20,20	0
6	MG	A	9442	1/1	0.99	0.05	-4.67	20,20,20,20	0
6	MG	C	9316	1/1	0.99	0.05	-4.77	20,20,20,20	0
6	MG	C	9239	1/1	0.99	0.04	-4.82	20,20,20,20	0
6	MG	D	9208	1/1	1.00	0.10	-5.14	20,20,20,20	0
6	MG	C	9243	1/1	0.99	0.06	-5.17	20,20,20,20	0
6	MG	C	9501	1/1	0.99	0.06	-6.49	20,20,20,20	0
6	MG	D	9203	1/1	0.99	0.08	-9.42	25,25,25,25	0
6	MG	A	9437	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9554	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	C	9514	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9383	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9337	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9469	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9421	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	A	9318	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9465	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	A	9368	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9390	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9504	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9285	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9265	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	A	9423	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9342	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	F	9463	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9533	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9496	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9398	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9450	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9348	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9393	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.09	-	20,20,20,20	0
6	MG	C	9359	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9356	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9325	1/1	0.99	0.10	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9444	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9434	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	A	9273	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9295	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9257	1/1	0.97	0.06	-	20,20,20,20	0
6	MG	C	9378	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	C	9320	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	A	9517	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	E	9373	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9331	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9426	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9301	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	C	9451	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9546	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	F	9414	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9385	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	E	9415	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9333	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	F	9298	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9440	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9304	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9526	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9552	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9332	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9443	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9489	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	E	9494	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	A	9487	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9222	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9472	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	E	9431	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9518	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9309	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9558	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9491	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.04	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9430	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9488	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9512	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9271	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	E	9484	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9290	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	F	9516	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	M	9206	1/1	0.97	0.10	-	38,38,38,38	0
6	MG	D	9461	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9305	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9456	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9548	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9272	1/1	0.97	0.07	-	20,20,20,20	0
6	MG	D	9406	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9529	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9340	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9202	1/1	0.96	0.07	-	43,43,43,43	0
6	MG	B	9541	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9269	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9483	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9330	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9327	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9454	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9306	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	B	9311	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9258	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9328	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9530	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	D	9506	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9334	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9241	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9361	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9323	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9445	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.07	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9513	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9477	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9503	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	C	9299	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9479	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9428	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	D	9372	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9497	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9297	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9562	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9261	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9400	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	F	9326	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	N	9205	1/1	0.99	0.08	-	16,16,16,16	0
6	MG	D	9214	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9336	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	F	9382	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	F	9425	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9217	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9286	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9403	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9338	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	C	9364	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	A	9464	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9395	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9490	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9474	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9384	1/1	0.96	0.07	-	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.09	-	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9355	1/1	0.98	0.13	-	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	E	9551	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9363	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9216	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	D	9362	1/1	0.99	0.05	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9371	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9370	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9561	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9291	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9460	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	D	9439	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9226	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	E	9538	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9470	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9267	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9547	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	B	9280	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9448	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	D	9559	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9410	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	B	9458	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9495	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9391	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9405	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9240	1/1	0.96	0.08	-	20,20,20,20	0
6	MG	D	9416	1/1	0.96	0.08	-	20,20,20,20	0
6	MG	D	9344	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9317	1/1	0.99	0.12	-	20,20,20,20	0
6	MG	A	9365	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9486	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9369	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9315	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9377	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9519	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	C	9358	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9467	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9367	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9407	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9399	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9223	1/1	0.99	0.09	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9536	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9528	1/1	0.97	0.06	-	20,20,20,20	0
6	MG	D	9296	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9446	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9485	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9452	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9505	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9354	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9375	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9475	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9520	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9293	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9250	1/1	0.97	0.06	-	20,20,20,20	0
6	MG	D	9248	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	C	9255	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	F	9424	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9478	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9466	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9441	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	D	9417	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9345	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	D	9308	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	F	9508	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9515	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9381	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9201	1/1	0.97	0.11	-	30,30,30,30	0
6	MG	D	9498	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9404	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9532	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	C	9524	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9468	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9413	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9324	1/1	1.00	0.07	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9339	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9527	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9357	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9453	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	F	9310	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9542	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9556	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	C	9511	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9394	1/1	0.97	0.09	-	20,20,20,20	0
6	MG	C	9476	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9409	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9246	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	E	9389	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9279	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9204	1/1	0.96	0.05	-	38,38,38,38	0
6	MG	D	9314	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9502	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	B	9256	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	E	9249	1/1	0.98	0.09	-	20,20,20,20	0
6	MG	D	9499	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	D	9539	1/1	0.99	0.03	-	20,20,20,20	0
6	MG	C	9422	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9531	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9252	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9433	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	E	9449	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9401	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	N	9207	1/1	1.00	0.08	-	37,37,37,37	0
6	MG	D	9510	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	C	9289	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9482	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9219	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	E	9341	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9545	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	A	9212	1/1	0.99	0.07	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9540	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9550	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9313	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	F	9500	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	D	9274	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9237	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9387	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9481	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9321	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9543	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	F	9245	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	E	9352	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	A	9555	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9351	1/1	1.00	0.09	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.